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**A COMPUTER MODEL FOR THE CALCULATION
OF THERMODYNAMIC PROPERTIES OF WORKING FLUIDS
OF A GAS TURBINE ENGINE**

**ENGINE TEST FACILITY
ARNOLD ENGINEERING DEVELOPMENT CENTER
AIR FORCE SYSTEMS COMMAND
ARNOLD AIR FORCE STATION, TENNESSEE 37389**

March 1976

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Prepared for

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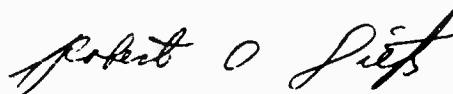
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This technical report has been reviewed and is approved for publication.

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20. ABSTRACT (Continued)

fuels and includes real gas effects (intermolecular forces and chemical dissociation). Equations for the thermodynamic properties of the constituents of air and exhaust gas are included. Calculated data from this program are compared with data from sources currently in use in the gas turbine industry.

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PREFACE

The research reported herein was conducted by the Arnold Engineering Development Center (AEDC), Air Force Systems Command (AFSC), under Program Element 65807F. The results of the research were obtained by ARO, Inc. (a subsidiary of Sverdrup & Parcel and Associates, Inc.), contract operator of AEDC, AFSC, Arnold Air Force Station, Tennessee, under ARO Project Numbers RF217 and RF414. The author of this report was John M. Pelton, ARO, Inc. Data analysis was completed on June 30, 1974, and the manuscript (ARO Control No. ARO-ETF-TR-75-92) was submitted for publication on June 25, 1975.

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1.0 INTRODUCTION

At the present time, the gas turbine engine industry has no generally accepted set of thermodynamic properties for the constituents of the working fluids or method for making thermodynamic calculations. Therefore, each segment of the industry from manufacturer through user may use slightly different basic thermodynamic data and calculation methods to arrive at the thermodynamic properties. The present condition is similar to that which existed in the rocket motor industry prior to the work of the ICRPG (Ref. 1) in establishing methods for performance calculations and data reduction.

As the operating environment of gas turbine engines has gone to higher temperatures and Mach Numbers, the differences in performance of competitive engines are often quite small. In fact, some performance differences are of the same order of magnitude as the change that may be expected from using different sets of thermodynamic properties of the constituents in the working fluids. Also because of the increased interaction between the engine and other components of the airframe, the need for a consistent method of arriving at thermodynamic properties becomes even more important. The increased use of mathematical models for describing engine performance has also increased the need for the use of consistent thermodynamic properties of the working fluids.

The gas turbine industry has developed from industries with diverse backgrounds and each segment has developed calculation procedures based on its own past history and present needs. The appearance of the computer as a routine tool for turbine engine analysis in even the smallest operation now provides the possibility for use of a consistent set of thermodynamic properties by all segments of industry and government if the properties can be coded for use with small computer memory and calculation times.

In an effort to develop a consistent thermodynamic model, certain guidelines were set up as follows:

1. Accessible constituents and constituent properties that are readily located so that orderly updating is possible as compositions for standard air and fuel change or thermodynamic property data are improved,

2. Acceptable memory requirements and calculation times for use in on-line data reduction systems, and
3. Contains real gas effects.

Certain items are required in such a consistent model, and these are identified below:

1. The composition of air,
2. The composition of hydrocarbon type fuels,
3. A set of thermodynamic properties for the constituents of working fluids, including real gas effects, and
4. A method of computing the thermodynamic properties of air and exhaust gas, including real gas effects.

Each of the above items was examined by reviewing the available literature and the present turbine industry usage in conjunction with the available computer technology for on-line data reduction calculations.

The pressure-temperature regime for air as a working fluid is shown in Fig. 1. The regime is from 0.1 to 600 psia and from 300 to 1,800°R. These limits were determined from current and projected future requirements for air as a working fluid in turbine engines. A number of air compositions were reviewed. They include the work of Self (see Edmunds, Ref. 2) and Keenan and Kaye (Ref. 3), Hilsenrath, et al. (Ref. 4), Touloukian (Ref. 5), Banes (Ref. 6), Brahinsky and Neal (Ref. 7), Brown and Warlick (Ref. 8), and the U.S. Standard Atmosphere (Ref. 9).

The composition of the hydrocarbon fuel was defined as C_nH_{xn} where "x" would be determined by the particular grade fuel in use.

There is a very limited amount of thermodynamic data from a single source that covers the necessary pressure and temperature regime for the air and exhaust gas constituents. The regime for air has been shown in Fig. 1, and the regime for exhaust gas is shown in Fig. 2. The regime for the exhaust gas is from 0.1 to 600 psia and from 600 to 4,000°R. The fuel-to-air ratio (f) to be considered will be from zero to stoichiometric. These model limits were based on current and projected future requirements for calculating exhaust gas thermodynamic properties in the turbine engine industry. Because of the overlapping of air and exhaust gas constituents such as nitrogen,

oxygen, carbon dioxide, argon, and neon, the temperature range for these constituents will be from 300 to 4,000°R. Constituents such as water vapor require thermodynamic properties from 600 to 4,000°R, while the products of chemical dissociation require thermodynamic properties from approximately 2,000 to 4,000°R. The two most complete sources of properties are JANAF (Ref. 10) and McBride, et al. (Ref. 11). Other sources reviewed included Hilsenrath (Ref. 4), Touloukian (Ref. 5), Din (Ref. 12), and Stull (Ref. 13). None of these sources was complete in terms of required constituents, temperature range or recent review and updating, but the JANAF data (Ref. 10) were chosen because of the temperature range and the on-going work in up-dating the data as more information becomes available. Two constituents, argon and neon, are not included in these tables; therefore data from Ref. 11 were used.

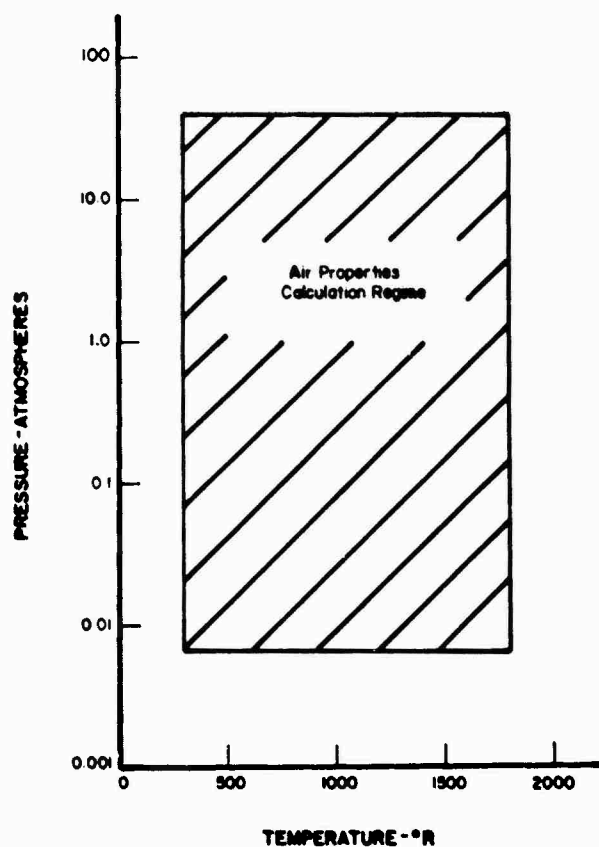


Figure 1. Pressure-temperature regime for the calculation of air properties.

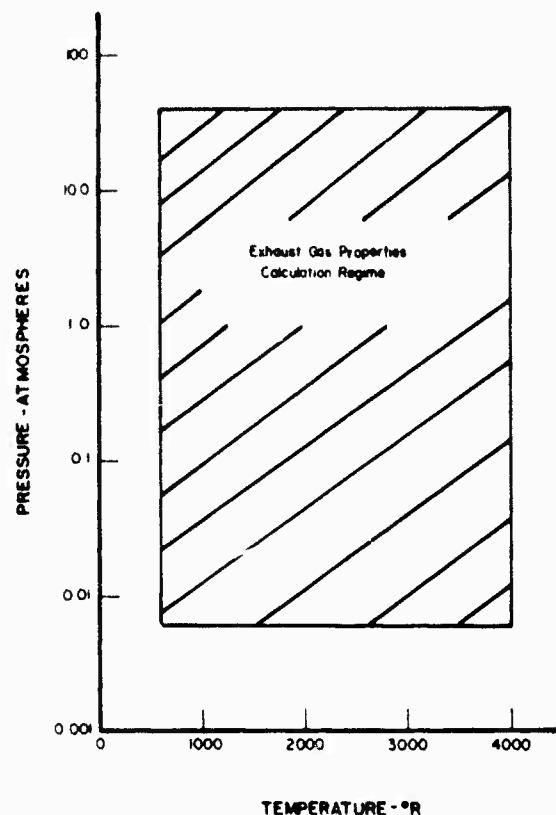


Figure 2. Pressure-temperature regime for the calculation of exhaust gas properties.

The real gas effects considered were intermolecular forces, chemical dissociation, vibrationally frozen flow, and ionization. The effects of intermolecular forces on the constituents of air are important and are developed in more detail in Section 2 as well as the effects of chemical dissociation in the exhaust gas. Chemical dissociation of air was considered, but the upper temperature limit was below the value where dissociation becomes important. A series of calculations were performed to determine whether vibrationally frozen flow should be included in the thermodynamic model. The results (Ref. 14) indicated that conditions would be highly unlikely to occur in a gas turbine engine where these types of losses would be considered significant. Ionization of air and exhaust gas was considered, but since the maximum exhaust gas temperature (4000°R, Fig. 2) is below the temperature where ionization becomes significant (Ref. 15), no corrections were included.

A number of methods for computing thermodynamic properties of exhaust gases are available for computer use. They fall into two general categories; one contains tabulated combustion properties, while the other is a computer program that calculates the properties. Examples of the former data format include Keenan and Kaye (Ref. 3), Banes, et al. (Ref. 6), and Powell, et al. (Ref. 16). Examples of the latter include Pinkel and Turner (Ref. 17), Osgerby and Rhodes (Ref. 18), and Gordon and McBride (Ref. 19). The use of the tabular form of pre-calculated data using some form of curve-fitting was rejected because of the desire to retain control over the air and fuel composition and thermodynamic properties of the constituents without having to recalculate the tables.

The thermodynamic model must be developed for on-line data reduction use, which means that calculation times and computer memory requirements must be minimized, but sufficient accuracy must be retained in the constituent property data so that the errors in the calculated values are not of the same size as the error in the experiment. The maximum time per calculation (temperature and pressure known, to calculate enthalpy, entropy, or specific heat) should be in the range of 0.05 sec and the memory requirements should be in the range of 10,000 words. By assuming the engine measurement error to be approximately one percent, the desired error between the original thermodynamic data for the constituents and the data calculated for use in the model should not exceed 0.1 percent (2 standard deviations).

This report describes a computer model developed to calculate the thermodynamic properties of the working fluids of a turbine engine. The model calculates the thermodynamic properties of air and the exhaust gas from the reaction of air with a hydrocarbon fuel. Composition of the air and fuel used with this model is discussed. The necessary thermodynamic properties of the constituents are presented as curve fits of the data from Refs. 10 and 11. The logic involved in the model is discussed as well as the method of operation. Calculated thermodynamic data from this model are compared with various data currently in use. A listing of the model is included.

2.0 DEVELOPMENT OF THE GENERAL COMPUTER MODEL

The computer model calculates the thermodynamic properties (enthalpy, entropy, specific heat, and Gibbs free energy) for the constituents of the working fluids of a turbine engine, air and exhaust gas.

In addition, the model calculates the enthalpy, entropy, specific heat, sonic velocity, and ratio of specific heats for air and exhaust gas. The model will determine the composition and molecular weight of the exhaust gas, but these two quantities are fixed for air.

The model is divided into two sections, the calculation of the air properties and the exhaust gas properties. The calculation of the air properties includes a correction for intermolecular forces of the constituents. The calculation of the exhaust gas properties includes the effects of chemical dissociation at high temperatures. A schematic of the calculation process for the model is shown in Fig. 3.

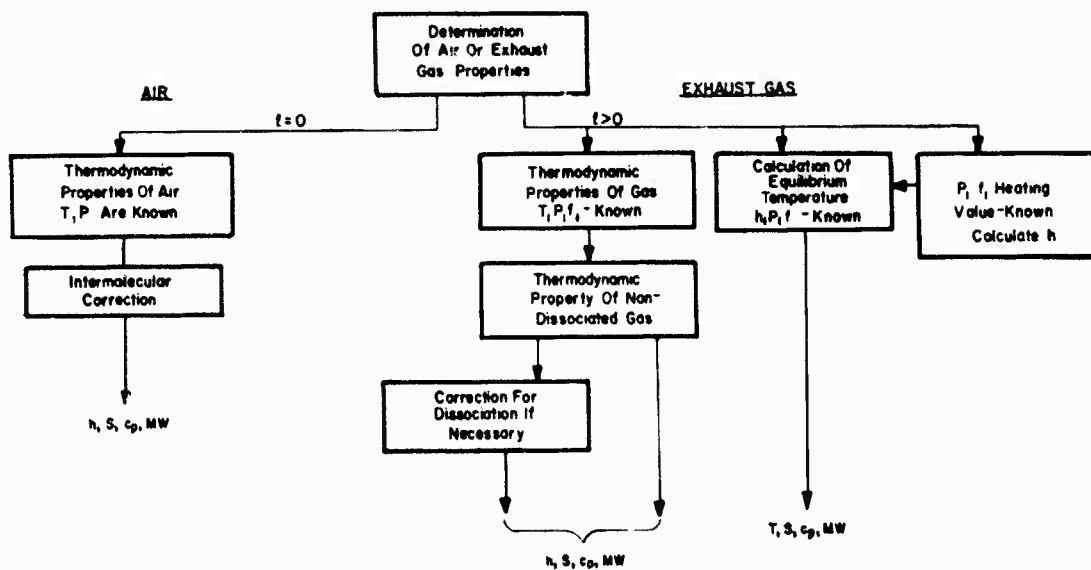


Figure 3. Schematic of computer model.

2.1 CALCULATION OF THE THERMODYNAMIC PROPERTIES OF DRY AIR

2.1.1 Composition and Molecular Weight of Dry Air

The composition of air is based on the U.S. Standard Atmosphere of Ref. 9. This composition was selected because of the detailed research that went into its original development and the ongoing work that can be used to update the composition if this becomes necessary. This particular source is also widely accepted in the turbine engine and related industries.

The composition of Ref. 9 contains seventeen constituents (see Table 1). To lessen storage requirements and computation time, the number of trace constituents was reduced. The criteria for reducing the number of constituents are listed below:

1. The molecular weight of the final composition would not deviate more than ± 0.010 percent from the value in Ref. 9 (28.9644 lbm/lbm-mole).
2. If the number of constituents necessary to meet item 1 is equal to or greater than three, the monatomic trace elements will be included with a Noble gas and the remaining trace constituents included with one of the other molecular constituents.

Using a four constituent composition (N_2 , O_2 , A, and CO_2) gives a molecular weight of 29.9651 if the monatomic elements are included with argon and the remainder with carbon dioxide. This molecular weight exceeds the 0.010-percent criteria and was rejected. A five constituent composition (N_2 , O_2 , A, CO_2 , and Ne) gives a molecular weight of 28.9646 lbm/lbm-mole if the remaining monatomic constituents are included with neon, and the other constituents are included with the carbon dioxide. A summary of the composition is shown below:

Constituent	Mole Fraction, n_i	Constituent Molecular Weight, MW_i	n_i , MW_i
Nitrogen	0.78084	28.0134	21.8740
Oxygen	0.209476	31.9988	6.7030
Argon	0.00934	39.944	0.3731
Carbon Dioxide (+ trace Constituents)	0.0003194	44.00995	0.0141
Neon (+ monatomic trace constitu- ents)	<u>0.0000246</u>	20.183	<u>0.0005</u>
	1.0000		28.9646

The molecular weight of this composition differs from that in Ref. 9 by 0.0002 or approximately 1 part in 150,000. Also the trace

constituents that have to be included with the five constituents amount to 0.00001182 percent.

The computer model considers this composition and molecular weight as fixed. If either the composition or molecular weight of one of the constituents were to change significantly, a simple card change would update the parameters. The inclusion of water vapor can also be made as a constituent of air.

2.1.2 Equations for the Calculation of the Thermodynamic Properties of the Constituents

The thermodynamic properties of primary interest are enthalpy, entropy, and specific heat at constant pressure. The properties of the constituents are taken from Refs. 10 and 11. The base temperature for enthalpy is taken as 0°R, and the reference pressure for entropy is one atmosphere. The tabular data from these sources were put into equation form for computer solution. The overall range of the data is from 300 to 1,800°R, and the data were divided into two ranges: from 300 to 900°R and from 900 to 1,800°R. The type equation chosen for the data and its degree was based on keeping the error between the original and the calculated data less than 0.1 percent (2 standard deviations). Attempts were made to fit the data to simple polynomial equations such as

$$a_i + b_i T + c_i T^2 + d_i T^3 + e_i T^4$$

$$\frac{1}{a_i + b_i T + \dots + e_i T^4}$$

and

$$\frac{a_i + b_i T + \dots + e_i T^4}{f_i + g_i T + \dots + h_i T^4}$$

The data in the low temperature range could not be fitted to the above type equations and meet the accuracy requirements; therefore a special technique discussed in Ref. 20 was used. This particular method gives the exact value at the tabulated points. Since Ref. 10 is tabulated in 180°R increments, additional data were requested from the source (Ref. 10) in 18-deg increments to provide a smoother curve fit. The data in the 900 to 1,800°R were fitted using the simple polynomial expressions given below:

Enthalpy

$$H_i = a_{ij} + b_{ij}T + c_{ij}T^2 + d_{ij}T^3 + e_{ij}T^4 \quad (1)$$

Entropy

$$S_i = a_{ik} + b_{ik}T + c_{ik}T^2 + d_{ik}T^3 + e_{ik}T^4 \quad (2)$$

Specific Heat

$$C_{p_i} = a_{in} + b_{in}T + c_{in}T^2 + d_{in}T^3 + e_{in}T^4 \quad (3)$$

The polynomial curve fit equations were generally third degree or less. The polynomial equations for the constituents of air will be found in Table 2 (900 to 1,800°R range). The fit of the original JANAF data for the major constituents gave a maximum error (2 standard deviations) of 0.1 percent when the data are recalculated for use in the computer model. Special precautions were taken to prevent a step from occurring in the properties at the transition region at 900°R.

2.1.3 Calculation of the Properties of Air

The calculation of the enthalpy, entropy, and specific heat (C_p) is made by summing the properties of the individual constituents based on their mole fractions in air. The equations used are:

Enthalpy:

$$H_{air} = \sum_{i=1}^5 n_i H_i \quad (4)$$

Entropy:

$$S_{air} = \sum_{i=1}^5 \left[n_i S_i - R_i \ln \left(\frac{P_i}{P} \right) \right] \quad (5)$$

Specific Heat:

$$C_{p_{air}} = \sum_{i=1}^5 n_i C_{p_i} \quad (6)$$

The mole fractions of the individual components of air (n_i) and the properties of these individual components are discussed in Section 2.1.1 and 2.1.2, respectively.

2.1.4 Correlation for Intermolecular Forces

Intermolecular forces produce a significant effect on thermodynamic properties of gases at higher pressures and lower temperatures. This effect can be seen in Fig. 4 where a nondimensionalized form of the specific heat at constant pressure (c_p/R) of air (from Ref. 4) is compared as a thermally perfect gas and real gas. The perfect gas property is calculated from spectroscopic data, and a virial correction is applied to this for the real gas property. In Fig. 4, the influence of pressure can be seen as the value of c_p/R increases as the pressure increases at the lower temperatures. To ensure that the calculated values of enthalpy, entropy, and specific heat for air in this model (Eqs. (4), (5), and (6)) include the effect of intermolecular forces, a correction is added to the calculation of these properties

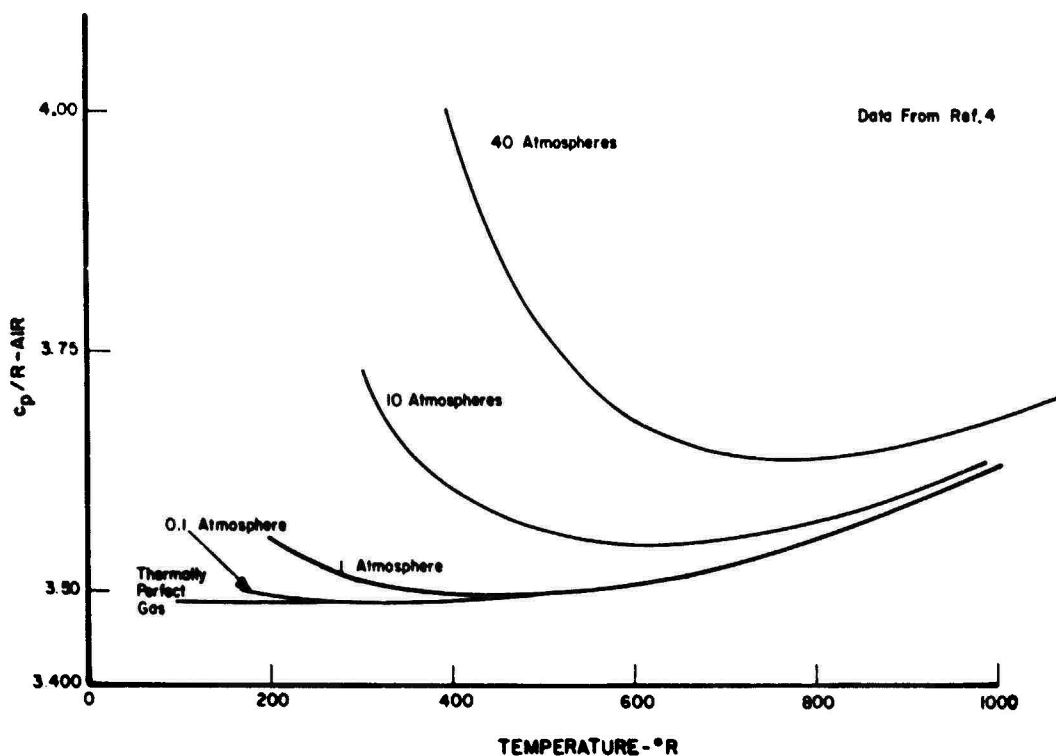


Figure 4. Effect of pressure on a nondimensionalized specific heat (c_p/R) for air at low temperatures.

for each of the constituents in air. The constituent corrections are then added to the properties calculated by Eqs. (1), (2), and (3). These corrected constituents are then summed according to Eqs. (4), (5), and (6) to get the properties of air at the particular temperature and pressure.

The equations for calculating the correction are taken from Ref. 21 and are given below:

Enthalpy:

$$H_{\text{correction}_i} = R_i T \left\{ \frac{1}{V_i} \left[B_i - T \frac{dB_i}{dT} \right] + \frac{1}{V_i^2} \left[C_i - \frac{T}{2} \frac{dC_i}{dT} \right] \right\} \quad (7)$$

Entropy:

$$S_{\text{correction}_i} = -R_i \left\{ \frac{T}{V_i} \frac{dB_i}{dT} + \frac{1}{2V_i^2} \left[B_i^2 - C_i + T \frac{dC_i}{dT} \right] \right\} \quad (8)$$

Specific Heat:

$$C_{p\text{correction}_i} = -R_i \left\{ \frac{T^2}{V_i} \frac{d^2B}{dT^2} - \frac{1}{V_i^2} \left[\left(B_i - T \frac{dB_i}{dT} \right)^2 - C_i + \frac{dC_i}{dT} - \frac{T^2}{2} \frac{d^2C_i}{dT^2} \right] \right\} \quad (9)$$

These corrections are then added to the value of the thermodynamic property calculated according to Eqs. (1), (2), and (3) as given below:

Enthalpy:

$$H_i = H_i + H_{\text{correction}_i} \quad (10)$$

Entropy:

$$S_i = S_i + S_{\text{correction}_i} \quad (11)$$

Specific Heat:

$$C_{p_i} = C_{p_i} + C_{p\text{correction}_i} \quad (12)$$

The (virial) coefficients and their derivatives for use in Eqs. (7), (8), and (9) were taken from data in Ref. 22. These data were fitted to polynomial equations for ease of calculations. The equations are given in Tables 3 and 4.

2.1.5 Summary of Air Properties and Equations

A five-constituent air is defined and shown below:

<u>Constituent</u>	<u>Mole Fraction</u>
Nitrogen	0.78084
Oxygen	0.209476
Argon	0.00934
Carbon Dioxide	0.0003194
Neon	0.0000246

The molecular weight is 28.9646. The thermodynamic properties of the air (enthalpy, entropy, and specific heat at constant pressure) are calculated from a summation of the properties of the constituents based on the composition ($\sum n_i H_i$, etc.). The constituent properties are curve fits of the data from Refs. 10 and 11. The data are fitted over a range from 300 to 1,800°R using the spline fit technique of Ref. 20 for the 300 to 900°R range and polynomial curve fits

$$a_{ij} + b_{ij}T + c_{ij}T^2 + d_{ij}T^3 + e_{ij}T^4$$

from 900 to 1,800°R. A correction for intermolecular forces (Eqs. (7), (8), and (9)) is added to thermodynamic properties calculated from Refs. 10 and 11. The equations for the constituent properties 900 to 1,800°R range and virial coefficients will be found in Tables 2, 3, and 4.

2.2 CALCULATION OF THE THERMODYNAMIC PROPERTIES OF TURBINE EXHAUST GAS

The model for calculating thermodynamic properties of exhaust produced from the combustion of a hydrocarbon fuel (C_nH_{xn}) and air consists of:

1. Determining the exhaust gas composition,

2. Calculating the thermodynamic properties of the constituents of the exhaust, and
3. Summing the constituent properties based on the mole fraction of constituent present in the exhaust gas.

The primary thermodynamic properties calculated are enthalpy, entropy, specific heat at constant pressure, and molecular weight. In addition, properties such as the ratio of specific heats and the sonic velocity are available as options.

The calculations can be made over a temperature range from 600 to 4,000°R, a pressure range from 0.1 to 600 psia, and fuel-to-air ratios from zero to stoichiometric (Fig. 2). The method of calculation is dependent upon whether the effects of chemical dissociation are included. The criteria for determining whether the effects of chemical dissociation are included are based on the dissociation of the oxygen molecule and are similar to the criteria of Ref. 23. If the following equation is true

$$T \geq T_I \quad (13)$$

where

$$T_I = 3000 + 182 \log P_a \quad (14)$$

then the effects of chemical dissociation of the exhaust gas are not considered. If

$$T < T_I \quad (15)$$

the effects of chemical dissociation are considered. Equation (14) is similar to the criteria of Ref. 24 and is based on the amount of dissociation in the oxygen molecule. When $T > T_I$, the mole fraction of the dissociated oxygen molecule will be 0.00500 or greater. Figure 5 shows the area of interest for the exhaust gas calculations with the division between the area where the effects of chemical dissociation are considered and not considered. This division has the benefit of removing most turbine calculations from the area where the effects of chemical dissociation are included.

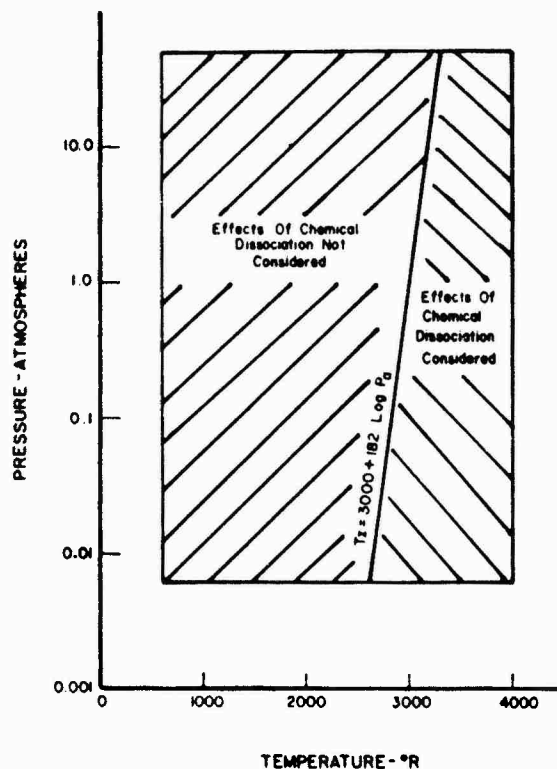
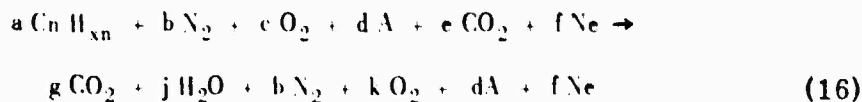


Figure 5. Pressure-temperature regime for the calculation of exhaust gas properties (considering dissociation).

The computer model for calculating the thermodynamic properties uses the air composition given in Section 2.1 and a hydrocarbon fuel composition of C_nH_{xn} . The fuel grade can be varied by suitable choice of "x" and by changing the hydrogen-to-carbon in the model. The thermodynamic properties of all constituents for air and exhaust gas are kept accessible in order that properties may be changed as new data become available.

2.2.1 Thermodynamic Properties of an Exhaust Gas with the Effects of Chemical Dissociation not Considered, $T \leq T_I$

The thermodynamic properties for an exhaust gas that is completely reacted with no effects of chemical dissociation considered are calculated for $T \leq T_I$. The assumed reaction and constituents involved are shown below:



The reaction is assumed to take place between:

$$600 \leq T \leq T_1 \quad (17)$$

The thermodynamic properties of the constituents in Eq. (16) will be found in Table 5. These data are curve fits of the tabular data found in Refs. 10 and 11 and cover the temperature range in Eq. (17). The method of making the exhaust gas calculations is basically the same as Refs. 17 and 25. The values of the thermodynamic properties h , s , c_p , and R of the exhaust gas are computed on the basis of the following assumptions:

1. The composition of the exhaust gas is based on the condition that the fuel is completely converted to CO_2 and H_2O . From this follows
 - a. The composition of the exhaust gas does not change in going through a thermodynamic process.
 - b. The amount of unburned hydrocarbons in the exhaust is negligible.
2. The internal energy states of each component gas are in equilibrium.
3. The exhaust gas behaves as a perfect mixture of perfect gases. Intermolecular forces are not considered.

As a result of assumption 3, the thermodynamic properties such as enthalpy of a mixed gas is the sum of the enthalpy of each component multiplied by the ratio of the mass of that component to the total mass of the mixture. For up to stoichiometric, the enthalpy of the exhaust gas is:

$$h_T = \left(\frac{1}{1+f} \right) \left[h_{\text{AIR}} + f \left(\frac{A^*m + B^*}{1+m} \right) \right] \quad (18)$$

where

$$A^* = \frac{h_{\text{H}_2\text{O}} - \frac{1}{2} h_{\text{O}_2}}{2.016} \quad (19)$$

$$B^* = \frac{h_{\text{CO}_2} - h_{\text{O}_2}}{12.011} \quad (20)$$

The term $[(A_m^* + B^*)/(1 + m)]$ in Eq. (18) accounts for the difference between the enthalpy of the water and carbon dioxide in the reacted mixture and the enthalpy of the oxygen removed from the air (h_{air}) by their formation. The term $[1/(1 + f)]$ expresses the units of mass of the enthalpy in terms of lbm of exhaust gas. A similar relation between the properties of the mixture and those of the constituent gases holds with regard to s , c_p , and R .

The molecular weight of the exhaust gas is determined by:

$$MW = \frac{Ru}{R} \quad (21)$$

2.2.2 Thermodynamic Properties of Turbine Exhaust Gas When the Effects of Chemical Dissociation are Considered, $T > T_I$

The calculation of thermodynamic properties at temperatures greater than T_I include the effects of chemical dissociation (see Fig. 5). In Section 2.2.1, the exhaust gas composition was defined as containing CO_2 , H_2O , and constituents of air. When chemical dissociation becomes important, the exhaust gas will contain numerous trace constituents. In addition to those shown in Eq. (16), the following are assumed as possible constituents: CO , H_2 , O , OH , H , and NO . Other constituents might be included, but the criteria were to eliminate any constituent whose mole fraction was less than 10^{-4} over the envelope shown in Fig. 2.

The calculation of a thermodynamic property such as enthalpy, entropy, or specific heat is made in two steps when the known value of temperature " T " is greater than T_I . The procedure is to calculate the sensible enthalpy at T_I by the method of Section 2.2.1, then to calculate the change in chemical plus sensible enthalpy going from T_I to T considering the exhaust gas to have a variable composition. The enthalpy change going from T_I to T is then added to the enthalpy at T_I to give the enthalpy at T .

The calculation of the thermodynamic property in the region from T_I to T where the composition is variable is done by the method of Ref. 13. The basic calculation method involves calculating the exhaust gas composition by the minimization of free energy. With the composition at T_I and T , the enthalpy is then calculated from the Eq. (22):

$$h_{(T,P)} = \frac{\sum_{i=1}^k n_i H_{i(T,P)}}{MW_{(T,P)}} \quad (22)$$

The enthalpy is also calculated at (T_I, P) :

$$h_{(T_I,P)} = \frac{\sum_{i=1}^k n_i H_{i(T_I,P)}}{MW_{(T_I,P)}} \quad (23)$$

The change in enthalpy is then the difference between Eqs. (23) and (22) and is the sensible component of the enthalpy difference:

$$\Delta h_{(T,P)} = h_{(T,P)} - h_{(T_I,P)} \quad (24)$$

The enthalpy calculated for the frozen composition at T_I by the method of Section 2.2.1 (Eq. (18)) is added to the sensible enthalpy of Eq. (24):

$$h_{(T,P)} = h_{(T_I)} + \Delta h_{(T,P)} \quad (25)$$

The calculated value of enthalpy is always a positive value. Using the method of Eq. (25) eliminates the problem of a discontinuity at T_I and there will be a smooth transition between the two calculation steps. The calculation for entropy and specific heat at constant pressure is made in the same manner. The calculation of the molecular weight is based on the composition calculated at T and P . The molecular weights summed as shown below:

$$MW_{(TP)} = \sum_{i=1}^k n_i MW_i \quad (26)$$

The thermodynamic properties of the various constituents needed for the model will be found in Table 5. These properties are polynomial curve fits of the data from Refs. 10 and 11. The equations are generally third degree or less.

2.2.3 Summary of Equations for the Calculation of Exhaust Gas Properties

A computer model was presented that calculates the thermodynamic properties of the exhaust gas formed from the reaction of air and hydrocarbon fuel (C_nH_{xn}). The model covers the temperature range from 600 to 4,000°R, the pressure range from 0.1 to 600 psia, and a fuel-to-air ratio from 0 to approximately stoichiometric. The model regime is divided into two calculation regions: one region where the exhaust gas is completely reacted into H_2O and CO_2 with no effects of chemical dissociation considered, and the region where the effects of dissociation are considered. The regions are divided by the equation (Eq. (14)):

$$T_I = 3000 + 182 \log P_a$$

which is based on the amount of molecular oxygen that dissociates in atomic oxygen.

The thermodynamic properties (h , s , c_p) for the exhaust with no effects of chemical dissociation considered are based on the method of Refs. 17 and 25. The equation (Eq. (18)) for calculating the enthalpy is:

$$h_T = \left(\frac{1}{1+f} \right) \left[h_{air} + f \left(\frac{A^* m + B^*}{1+m} \right) \right]$$

and the calculation for entropy, specific heat, and the gas constant follows the same format. The method for calculating the same properties in the region where the effects of chemical dissociation are considered uses a combination of the method given above and the method of Ref. 18. The property, enthalpy for instance, is calculated as a nondissociated gas at temperature T_I . The composition of the exhaust gas is then calculated at T and T_I (and the known pressure), and the enthalpy is calculated at the two temperatures based on the mole fraction of the various constituents. The difference in enthalpy at the two temperatures (T and T_I) is added to the nondissociated enthalpy calculated at T_I to give the enthalpy at the known temperature and pressure. The calculation of the entropy and specific heat follows the same format. The calculation of the molecular weight is based on a summation of the molecular weights of the constituents weighted by the mole fractions calculated at the known temperature and pressure.

The thermodynamic properties of the constituents are presented as curve fits of the tabular data found in Refs. 10 and 11.

3.0 OPERATION OF THE COMPUTER MODEL

The computer model calculates the thermodynamic properties of air and of the products of combustion of air and a hydrocarbon fuel ($C_n H_{Xn}$). The input parameters for the model are temperature ($^{\circ}R$), pressure (psia), fuel heating value (Btu/lbm), fuel-to-air ratio (lbm/lbm), exhaust gas enthalpy (Btu/lbm), and XKON (dimensionless control parameter). The normal calculation procedure is to solve for enthalpy, entropy, specific heat, and molecular weight when the temperature, pressure, and fuel-to-air ratio are known. The model will calculate the equilibrium exhaust gas temperature if the pressure, fuel-to-air ratio, and the exhaust gas enthalpy are known. The same calculation can be made if the fuel heating value is known instead of the exhaust gas enthalpy. The particular calculation is determined by the computer through the use of dummy input parameters. The general operation of the computer model and the specific model inputs will be described below. A general flow diagram of the program is shown in Fig. 3, and a listing will be found in Appendix B.

The model is divided into two sections, one calculates the air properties and the other calculates the exhaust gas properties. The model initially decides which section is required from the value of the fuel-to-air ratio (f). If the value is zero, then the calculation of thermodynamic properties is made for air; if a positive value is presented, then properties for exhaust gas are calculated (if by accident a negative value is input, the program prints an error message and the value of " f "). For the calculation of the thermodynamic properties of air, the required input data are the known value of air temperature and pressure and zero for the fuel heating value, fuel-to-air ratio, enthalpy, and XKON. With the value of " f " equal to zero, the program begins the calculation of air properties in subroutine THERMO where the molar composition of air is located as well as the molecular weights for the constituents of air and the fixed molecular weight of air. The thermodynamic properties of air are calculated in subroutine GAS, and the corrections for intermolecular forces are calculated in subroutines HMIXP, SMIXP, and CPMIXP. If the air temperature is between 300 and 900 $^{\circ}R$, the constituent properties of air are calculated in subroutine HSCP which is the special curve fitting routine of Ref. 20, and if the temperature is between 900 and 1800 $^{\circ}R$, the constituent properties are calculated from the polynomial curve-fits in subroutine COEFF.

The calculation of the thermodynamic properties of the exhaust gas follows a path similar to air. Typical required inputs are the known temperature, pressure, and fuel-to-air ratio and zero for the fuel heating value, enthalpy, and XKON. In this case, the positive "f" indicates that an exhaust gas calculation will be made and then a check is made to see if the temperature and pressure are in the area where the effects of chemical dissociation are included (Eq. (14) or Fig. 5). If the properties are in the nondissociated region subroutine GAS is called with temperature, and "f." The thermodynamic properties of exhaust gas are calculated in this subroutine using the individual constituent properties calculated from subroutine COEFF. If the required properties are in the dissociated region, the temperature, pressure, and "f" are used in subroutine CHEMEQ to set up the atom concentration of the individual constituents in the fuel and air. These concentrations and the temperature and pressure are used in subroutine PROP to solve for the equilibrium concentration of the exhaust gas species. Subroutine PROP contains the convergence criteria (DELL) which is currently set for 10^{-4} for N_2 and H_2O and 10^{-6} for O_2 . This means that the partial pressure of H_2O , N_2 , and O_2 must not change by more than 10^{-4} or 10^{-6} between successive iterations during the solving for the specie concentration. Generally a solution is achieved within three iterations. The thermodynamic properties such as Gibbs free energies are calculated in subroutine THERM from constituent properties found in subroutine COEFF. When the equilibrium concentration is established, then the thermodynamic properties like enthalpy, entropy, and specific heat are determined in subroutine THERM from constituent properties found in subroutine COEFF.

The model will also determine the equilibrium exhaust gas temperature for known values of pressure, enthalpy, and fuel-to-air ratio. Zero is input for the fuel heating value and XKON and +1.0 for the temperature. The data go through subroutine THERMO into CHEMEQ where the atom concentrations of oxygen, nitrogen, argon, neon, carbon, and hydrogen are determined and sent to subroutine PROP along with the pressure and enthalpy. Subroutine PROP contains an initial estimate of the temperature (currently set at 3,006°R) to be used to calculate the Gibbs free energy and ultimately a first estimate of the enthalpy. This enthalpy is compared with the known value of enthalpy, and a correction is made to the estimated temperature based on the difference in the enthalpies. An iteration loop is set up, and the temperature is changed until the partial pressure of H_2O , O_2 , and N_2 converge to meet the requirements of DELL discussed earlier and the temperature change is less than $(0.1)(c_p)$ or approximately 0.03°.

The model will also determine the equilibrium temperature if the heating value of the fuel is known. The input for this case would be pressure, fuel heating value, and fuel-to-air ratio. A value of -1.0 is input for the enthalpy and XKON and +1.0 for the temperature. The negative values have no physical meaning, but are used to direct the model to specific subroutines. The actual calculation procedure is the same as for the previous case where the enthalpy was known, except that the enthalpy of the fuel must be determined from the fuel heating value in subroutine FUELH. The convergence criteria for H₂O, O₂, and N₂ are the same as discussed earlier.

A subroutine (SONV) has been included with the program to calculate the ratio of specific heats and the sonic velocity. This subroutine uses inputs (molecular weight, fuel-to-air ratio, temperature, and the specific heat at constant pressure) from the main program, but the subroutine is not called automatically. Therefore, if these calculated values are required, call statements must be given in the subroutine where the values are required.

4.0 PRESENTATION OF RESULTS AND COMPARISON OF DATA

Various thermodynamic properties were calculated using the computer program of this report and were compared with other data currently in use in the turbine engine industry. The compared data consisted of enthalpy and specific heat at constant pressure for both air and turbine exhaust gas as the working fluid.

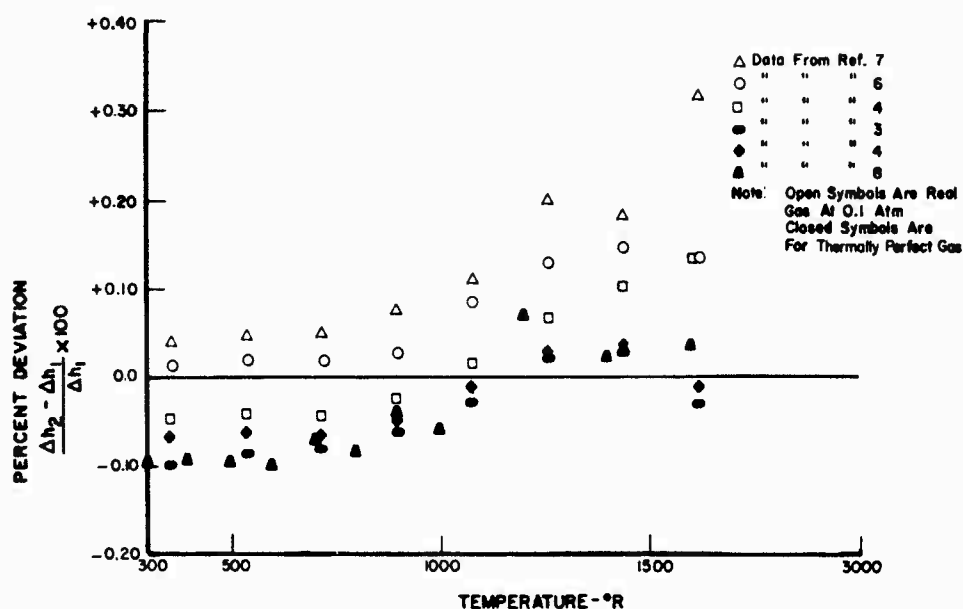
4.1 COMPARISON OF DATA FOR AIR

Enthalpy is a primary thermodynamic property used in the analysis of a turbine engine. The enthalpy of air based on the model described was compared with the published values of enthalpy in Refs. 3, 4, 6, 7, and 8. The enthalpy was compared by the percent deviation as a function of temperature. The percent deviation was calculated by

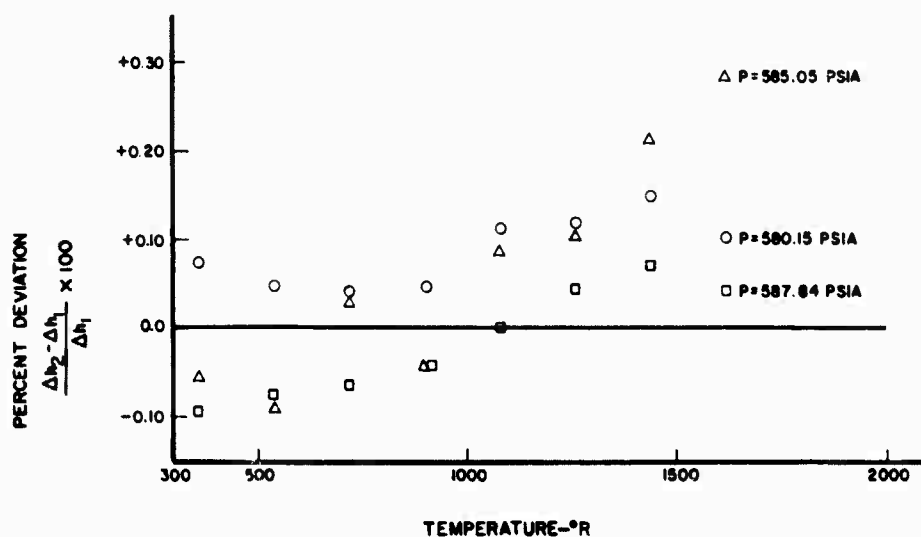
$$\text{Percent Deviation} = \frac{(h_B - h_T)_2 - (h_B - h_T)_1}{(h_B - h_T)_1} \times 100 \quad (27)$$

The data from the previously listed sources are noted ()₂ while the data calculated using the method of this report are noted by ()₁. Because of the different base temperatures for enthalpy and/or the constituent data an artificial base was used, and all data were compared as an enthalpy difference between the desired temperature and that of 1,800°R. The base temperature was chosen at 1,800°R because air can be treated as a thermally perfect gas at this temperature; also this is the maximum temperature for the air calculations. The data were compared at two pressures, a low pressure of 0.1 (Fig. 6a) and a high pressure of approximately 40 atm (Fig. 6b). Shown in Fig. 6a is a comparison of the data from this program with three sets of data where air is treated as a thermally perfect gas (Refs. 3, 4, and 8) and the enthalpy is a function of temperature only. In these references, there are no corrections for pressure, and the deviation between thermally perfect gas behavior and a real gas can be seen. Figure 6a shows that air properties as calculated by this program approach perfect gas behavior at 1,100°R. The data also show that the calculated enthalpy data are below that for a perfect gas above 1,100°R and are due to differences in composition and properties. Figure 6a shows a positive deviation for the data comparison with Refs. 6 and 7 which consider real gas effects. This deviation indicates that the term $(h_{1800} - h_T)_2$ is larger than the same value calculated by this program $(h_{1800} - h_T)_1$ and, therefore, shows that the correction for intermolecular forces in the two references is larger than the values used in this program. Figure 6b shows the data as calculated by this program for high pressures (approximately 40 atmosphere) to be very similar to the data in Refs. 4, 6, and 7. This means that the corrections for intermolecular forces are approximately the same at this pressure. The correction again becomes less for this program at 1,100°R.

Figures 7a and b compare the calculated value of specific heat at constant pressure (c_p) with that from Refs. 4 and 6. The first reference considers air as both a real gas and a thermally perfect gas, whereas the latter reference considers air only as a real gas. The deviations in both cases are generally less than 0.2 percent except for 40 atm where the deviation varies from -0.2 to -0.4 percent. The fact that the deviations are negative indicates that the calculated values of c_p are larger, and in this case, the larger value is due to the difference in air composition and constituent properties rather than the corrections. This can be seen from the fact that the thermally perfect gas c_p in Fig. 7a from Ref. 4 has a negative deviation of the same approximate value as the real gas c_p up to a pressure of 10 atm.

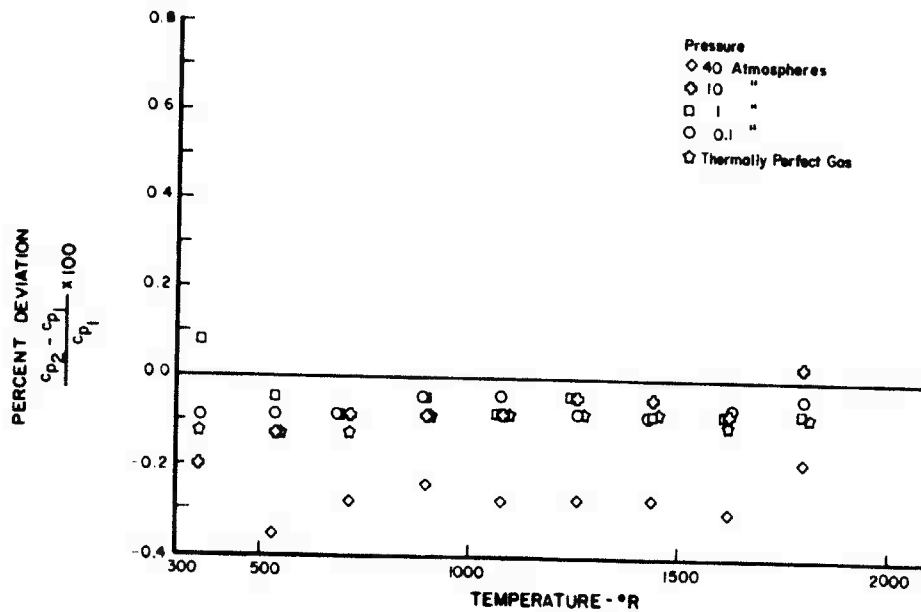


a. Low pressure (0.1 atm or as a thermally perfect gas)

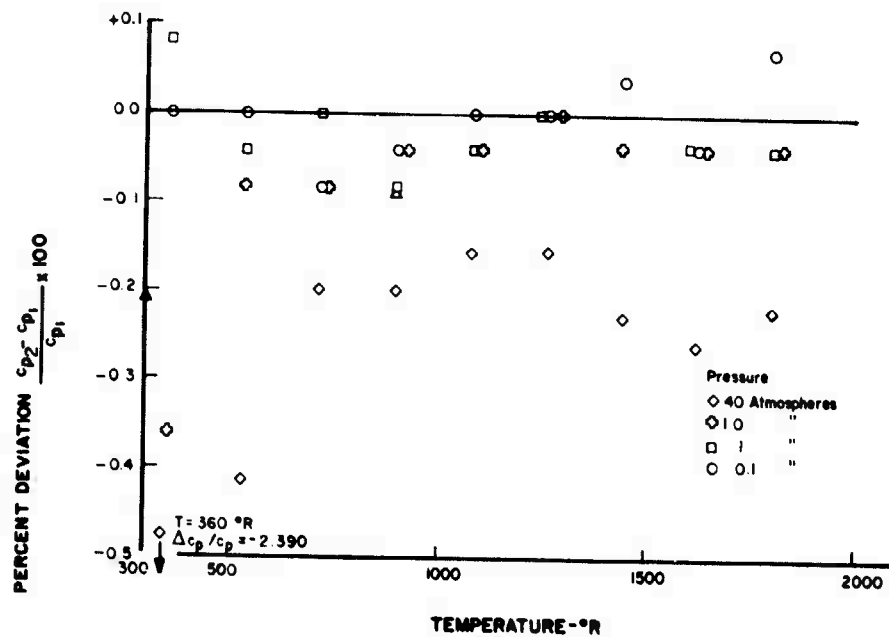


b. High pressure

Figure 6. Percent deviation in enthalpy of air as calculated by this program and compared with several sets of data in common use.



a. Data compared with that from Ref. 4



b. Data compared with that from Ref. 6

Figure 7. Percent deviation of the calculated value of c_p of air at several pressures and compared with data from Refs. 4 and 6.

A comparison of the deviation at 360°R and approximately 40 atm in Figs. 7a and b shows a large difference between the data of Refs. 4 and 6. This spread indicates the differences that can occur in various data sources at low temperatures and high pressures. In this area, the correction data used in this computer model places the calculated data in between these two sources and gives additional assurance that the correction terms are reasonable.

4.2 COMPARISON OF DATA FOR EXHAUST CALCULATIONS

4.2.1 Comparison of Data with Those in the Published Literature

The thermodynamic data calculated by this portion of the program were compared with similar data available in the published literature. The data comparison was made with enthalpy since it is a parameter of major importance in the data analysis of turbine engines. The comparison was presented in terms of percent deviation as calculated by Eq. (28).

$$\text{Percent Deviation} = \frac{(h_T - h_B)_2 - (h_T - h_B)_1}{(h_T - h_B)_1} \times 100 \quad (28)$$

The data were calculated in terms of enthalpy differences between the known temperature and the base temperature. The base temperature was 600°R when data from Ref. 15 were being compared and 540°R when data from Ref. 6 were used. To compare the data, fuel was assumed C_nH_{2n} to be consistent with the data in the references. This meant that the hydrogen-to-carbon atom ratio (M) in subroutine THERMO was set at 0.1678 ($2 \times 1.008/12.011$) and that the number of carbon atoms (XN) was set equal to 1.0 and the number of hydrogen atoms (XM) was set equal to 2.0 in subroutines CHEMEQ and MFNOD. Also in subroutine CHEMEQ, the stoichiometric ratio was defined as 0.067623 in the equation for PHI. The input data were

$$1000^\circ\text{R} \leq T \leq 4000^\circ\text{R}$$

$$p = 14.696 \text{ psia}$$

$$f = 0.067623 \text{ lbm}_{\text{fuel}}/\text{lbm}_{\text{air}}$$

Figure 8 shows the percent deviation versus temperature from the data of Refs. 6 and 16. The data show good agreement from 2,000 to 2,800°R. When the data from Refs. 6 and 16 include significant corrections for chemical dissociation (beginning at 2,800°R), the deviation begins to increase. This increase continues until the temperature $T = T_I$. This increase in deviation is caused by this model not considering dissociation at a lower temperature (i. e. 2,800°R). The deviation between 2,800 and 3,000°R (or the temperature that dissociation is considered in this program) becomes a constant bias for the rest of the data at higher temperatures. The presence of this bias is evident from Eq. (25) where the enthalpy at a high temperature (above T_I) is the sum of the enthalpy at the temperature T_I plus the difference in enthalpy between T and T_I . This is also born out in Fig. 8 where the deviation is shown to be essentially constant after reaching the temperature T_I (which is 3,000°R for these data). A second data comparison is shown in Fig. 9 for the same fuel composition and pressure, but the fuel-to-air ratio is now 0.033812. The agreement with the data from Ref. 17 is good, again showing the characteristic increase in deviation up to 3,000°R and then becoming

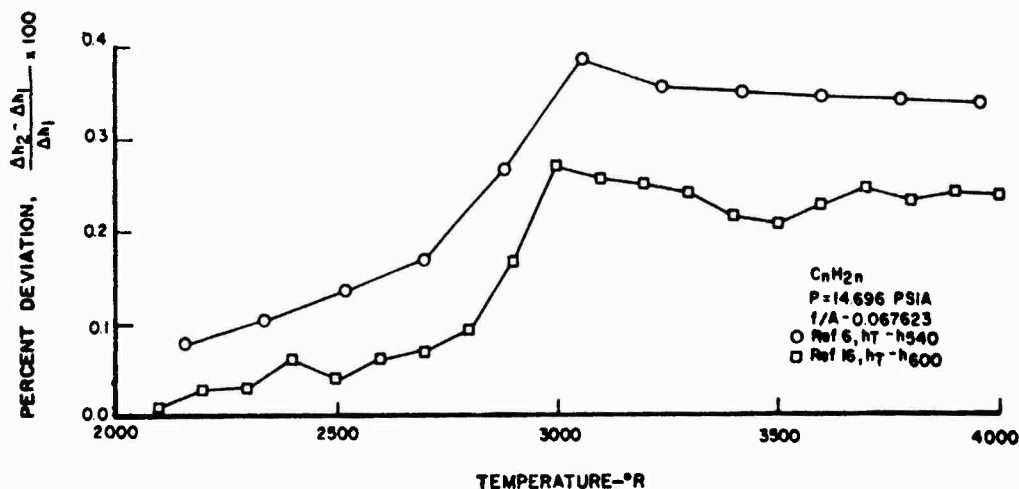


Figure 8. Percent deviation of the enthalpy of turbine exhaust gas as calculated by the method of this report and Refs. 6 and 16 at a fuel-to-air ratio of 0.067623.

essentially constant. The agreement with the data from Ref. 3 is good until the computer program begins to consider dissociation, and the agreement becomes very poor. The large deviations with the data from Ref. 3 are caused by this source not considering dissociation, and therefore, the enthalpy difference will be smaller in Eq. (28) and

leads to a negative deviation that gets progressively larger as the temperature increases.

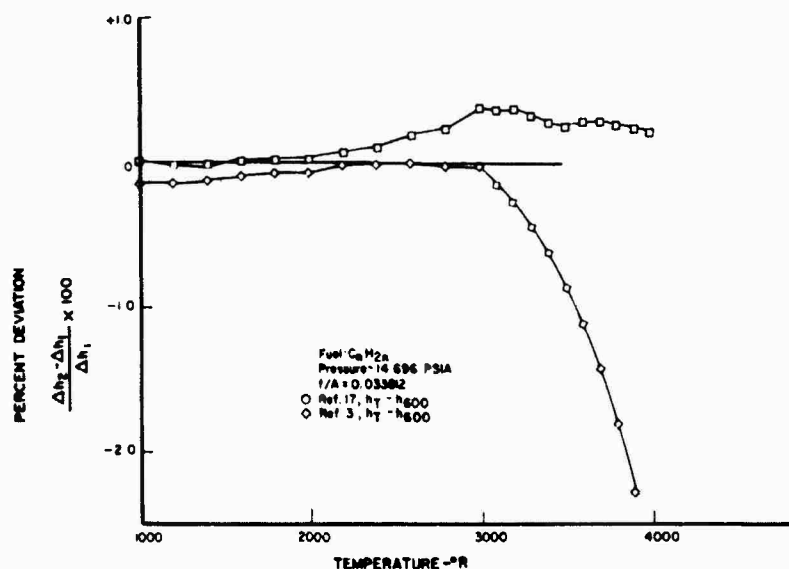


Figure 9. Percent deviation of the enthalpy of turbine exhaust gas calculated by the method of this report and Refs. 3 and 17 at a fuel-to-air ratio of 0.033812.

4.2.2 A Comparison of the Enthalpy of Two Hydrocarbon Fuel Compositions

A common hydrocarbon fuel grade in use in the gas turbine industry today is JP-4. Because it is a mixture of petroleum distillates, the chemical composition is hard to define. Generally, the average composition is around $C_nH_{1.95n}$ to $C_nH_{2.0n}$. To determine the order of difference in enthalpy that would occur because of a change in hydrogen-to-carbon atom ratio in the fuel, a series of calculations were made with each composition. The required computer parameters for $C_nH_{2.0n}$ were noted earlier, and those for the composition $C_nH_{1.95n}$ are

$m = 0.1636$ (in subroutine THERMO)
 $XN = 1.0$ (in subroutines CHEMEQ and MFNOD)
 $XM = 1.95$ (in subroutines CHEMEQ and MFNOD)
 Stoichiometric ratio = 0.06795 (in subroutine CHEMEQ)

The calculations were made at two pressures 14.696 and 1.4696 psia and at the stoichiometric fuel-to-air ratio. The results are presented in Fig. 10. The data show the deviation to be approximately constant at 0.12 percent. There is a slight additional deviation caused by the change in pressure from 14.696 to 1.4696 psia when the effects of dissociation are included, but this change is small when compared with the deviation caused by the fuel composition.

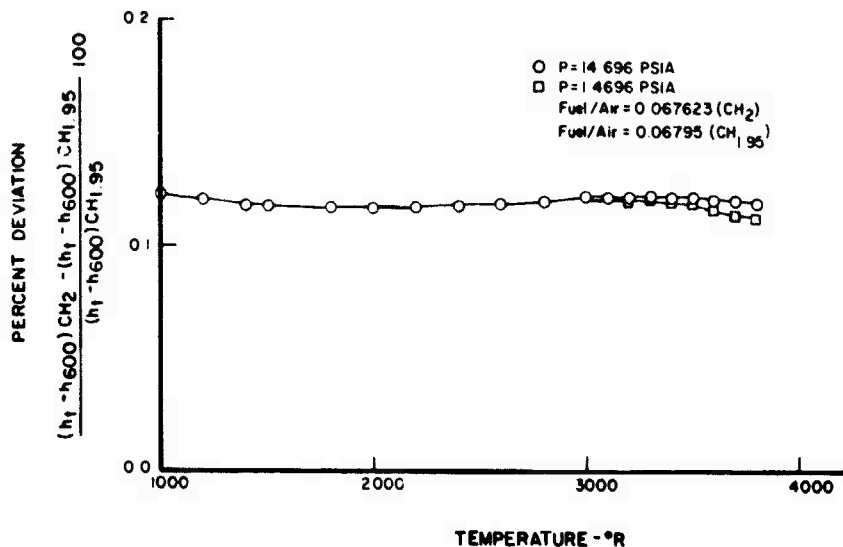


Figure 10. Percent deviation of the enthalpy as a function of temperature using a fuel composition of CH_2 and $\text{CH}_{1.95}$.

4.2.3 Effect of the Thermodynamic Model on the Calculation of Turbine Afterburner Efficiency

In recent years, there has been some variation in the chemical model used to determine turbine engine performance for the case of low efficiencies in afterburner tests. A comparison was made to determine if other suggested models made a significant difference in the calculated afterburner efficiencies. Accordingly, four models were investigated as follows:

1. No effects of chemical dissociation, but with prescribed proportions of CO ,
2. No effects of chemical dissociation but with prescribed quantities of unburned fuel (assumed to be CH_2) in the exhaust gas,

3. Complete chemical equilibrium, and
4. Complete chemical equilibrium, but with prescribed quantities of unburned fuel in the exhaust.

The method of comparing the thermodynamic models used by Dr. I. T. Osgerby for this study and the data are discussed in Appendix A. The results indicated that the chemical model considered had an insignificant effect on calculated afterburner efficiency. In addition, the data also showed that the calculated afterburner efficiency was not significantly altered by considering chemical dissociation in the exhaust gas stream as opposed to assuming that the fuel is completely converted to CO_2 and H_2O up to an exhaust gas temperature of $3,200^\circ\text{R}$.

4.2.4 Review of the Data for Internal Consistency

To determine the interval consistency of the computer program, two cross-checks were made using the thermodynamic properties, enthalpy, entropy, and specific heat of air and exhaust gas. One check of the data used the definition of c_p

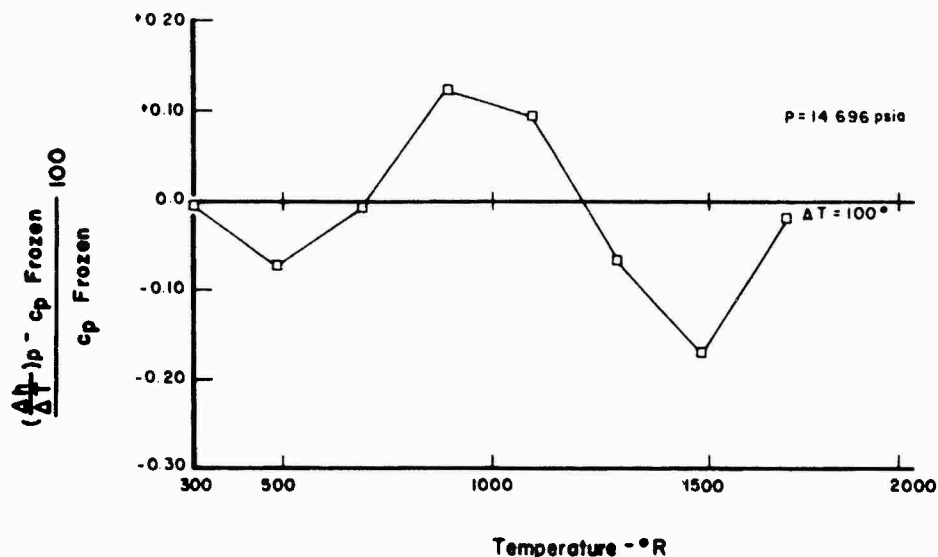
$$\left(\frac{\partial h}{\partial T}\right)_p = c_p \quad (29)$$

where the enthalpy of air and exhaust gas were calculated over a 100°R interval and compared with the specific heat calculated at the average temperature as shown below.

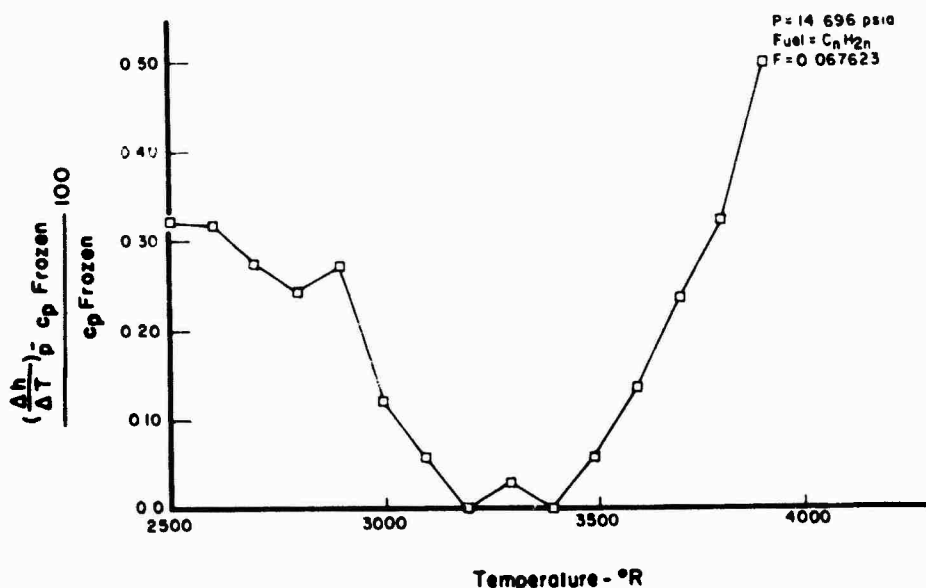
$$\frac{\left(\frac{h_{(T+100)} - h_T}{100}\right)_p - c_{p(T+100/2)}}{c_{p(T+100/2)}} \cdot 100 \quad (30)$$

The comparison for air and exhaust gas as a function of temperature is shown in Fig. 11. The data for air were calculated at 14.696 psia. Figure 11a shows an approximate deviation of ± 0.15 percent over the temperature range from 300 to $1,700^\circ\text{R}$. This deviation compares favorably with the maximum error of 0.1 percent allowed for the constituent properties. The deviation at 900°R indicates the approximate error caused by the numerical process since the curve fit of all the constituent properties is exact at this temperature. The same comparison was made for exhaust gas at an "f" of 0.067623 and 14.696 psia

in Fig. 11b. The deviation varies from +0.30 to -0.25 percent which is essentially the same as for the air. The comparison of the exhaust gas was made from 2,500 to 3,900°R. This temperature range covers both the dissociated and nondissociated range of compositions.



a. Deviation of air



b. Deviation of exhaust gas

Figure 11. $(\Delta h/\Delta T)_p$ compared with c_p as calculated by this computer model to measure internal consistency.

A second comparison was made to compare enthalpy and entropy of air and exhaust gas using the relationship:

$$\frac{1}{T} \left(\frac{\partial h}{\partial T} \right)_p = \frac{\partial s}{\partial T} \quad (31)$$

This relationship was used by calculating enthalpy and entropy over a 100°R temperature interval and calculating the deviation. The results are shown in Figs. 12a and b for air and exhaust gas, respectively.

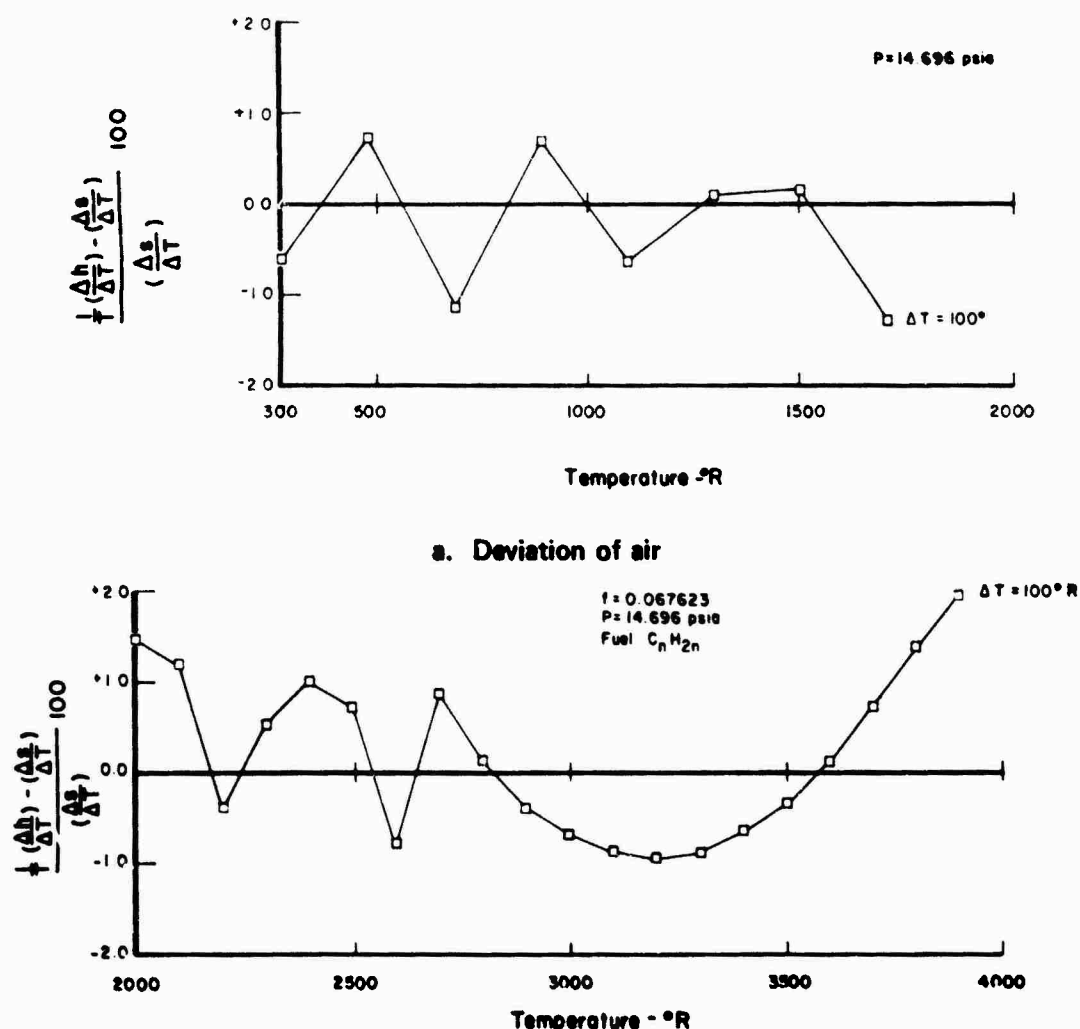


Figure 12. Deviation between the function $1/T (\Delta h/\Delta T)_p$ and $(\Delta s/\Delta T)$ as a function of temperature to determine the internal consistency of the computer program of this report.

The deviation for air is approximately ± 1 percent, and the maximum deviation for exhaust gas is approximately ± 1.5 percent. The deviation is believed to be caused by calculating a series of constituent properties and summing them rather than any inconsistency between the data for enthalpy and entropy. This is based on the calculated deviations shown in Fig. 12a between 300 and 900°R where the calculated constituent properties are in essentially exact agreement with Refs. 10 and 11, yet the sum of these properties for the air mixture shows a deviation from +0.75 to -1.1 percent. The data for the exhaust gas show a similar deviation, and by removing the end points, the deviations for the air and exhaust gas are similar. The size of the deviations is probably inherent in the calculation process and not a function of any internal inconsistencies in the basic data.

4.3 COMPUTER CALCULATION TIMES

One of the objectives of the program was to develop computer software that would not require excessive computer time. To determine the length of time required to make the various calculations, a time check was incorporated in the program. The time required to make the calculations (T , P , and f known with h , s , and c_p to be calculated) are listed below:

<u>Constituents</u>	<u>Time, sec</u>
Air (with intermolecular corrections)	0.009
Exhaust gas	
nondissociated	0.003
dissociated	0.028

These calculations were determined using an IBM 370/155 computer.

5.0 CONCLUSIONS

A computer model was developed to calculate the thermodynamic properties of air ($300^\circ\text{R} \leq T \leq 1800^\circ\text{R}$, $0.007 \text{ atm} \leq p \leq 40.8 \text{ atm}$, and the exhaust gas ($600^\circ\text{R} \leq T \leq 4000^\circ\text{R}$, $0.007 \text{ atm} \leq p \leq 40.8 \text{ atm}$, $0 \leq f/f_{\text{stoichiometric}} \leq 1.0$) of a turbine engine. The composition of the air was

<u>Constituent</u>	<u>Mole Fraction</u>
N ₂	0.78084
O ₂	0.209476
A	0.00934
CO ₂	0.0003194
Ne	0.0000246

and the fuel composition was C_nH_{xn} . Several real gas effects were investigated, and a correction for intermolecular forces was applied to the constituents of air. A correction for chemical dissociation was applied to the exhaust gas.

The thermodynamic data for the constituents of air and exhaust gas were taken from the JANAF tables (Ref. 10) and curve fitted for use in the computer model. The data as calculated for use in the model had a maximum error of 0.1 percent (2 standard deviations) when compared with the JANAF tabulations. The calculated enthalpy data for air were compared at 0.1 and 40 atm with NBS data (Ref. 4). The maximum deviations expressed as

$$\frac{(h_T - h_{1800^\circ})_{NBS} - (h_T - h_{1800^\circ})_{Model}}{(h_T - h_{1800^\circ})_{Model}} \times 100$$

were approximately -0.08 and -0.10 percent, respectively. The calculated enthalpy for a turbine exhaust gas (C_nH_{xn} /Air system at 14.696 psia and a fuel-to-air ratio of 0.0676) was compared with similar data from the AGARD tables (Ref. 6). The maximum deviation (expressed in a similar manner to air) was 0.4 percent.

A set of calculations was performed to see if the low efficiencies frequently experienced during afterburner testing could be traced to the chemical model employed. The data showed that, for all models considered, the calculated efficiencies were essentially the same.

Calculation times were determined for different type data. Typical times for a known T and P are listed below:

<u>Constituents</u>	<u>Time, sec</u>
Air (with intermolecular corrections)	0.009
Exhaust gas	
nondissociated	0.003
dissociated	0.028

These calculations were determined using an IBM 370/155 computer.

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Table 1. Air Composition from Ref. 9

<u>Constituent Gas</u>	<u>Content*, percent by volume</u>
1. Nitrogen (N_2)	78.084
2. Oxygen (O_2)	20.9476
3. Argon (Ar)	0.934
4. Carbon dioxide (CO_2)	0.0314
5. Neon (Ne)	0.001818
6. Helium (He)	0.000524
7. Krypton (Kr)	0.000114
8. Xenon (Xe)	0.0000087
9. Hyrdogen (H_2)	0.00005
10. Methane (CH_4)	0.0002
11. Nitrous oxide (N_2O)	0.00005
12. Ozone (O_3)	Summer: 0 to 0.000007 Winter: 0 to 0.000002
13. Sulfur dioxide (SO_2)	0 to 0.0001
14. Nitrogen dioxide (NO_2)	0 to 0.000002
15. Ammonia (NH_3)	0 to trace
16. Carbon monoxide (CO)	0 to trace
17. Iodine (I_2)	0 to 0.000001

*Numbers 1 through 11 are included in model;
 numbers 12 through 17 are assumed to be zero.

Table 2. Equations for the Thermodynamic Properties of the Constituents of Air

1. Equations for Sensible Enthalpy (BTU/lbm-mole)

1. Temperature Range 900°-1800°R

$$N_2, H = 272.57872 + 6.2849888T + 4.2460662 \times 10^{-4}T^2$$

$$O_2, H = -49.9253121 + 6.8005911T + 4.6097941 \times 10^{-4}T^2$$

$$A, H = 0.19368 + 4.9682152T$$

$$CO_2, H = -291.6316413 + 6.5377190T + 28.320187 \times 10^{-4}T^2 - 0.3858033 \times 10^{-6}T^3$$

$$Ne, H = 0.19368 + 4.9682152T$$

2. Equations for Entropy (less - $RLnp_i$ term), (BTU/lbm-mole, °R)

Temperature Range 900-1800°R

$$N_2, S = 39.251394 + 0.0155587T - 0.5615997 \times 10^{-5}T^2 + 0.933764 \times 10^{-9}T^3$$

$$O_2, S = 42.269726 + 1.5770590 \times 10^{-2}T - 0.5390427 \times 10^{-5}T^2 + 0.8573795 \times 10^{-9}T^3$$

$$A, S = 31.5883510 + 1.2918283 \times 10^{-2}T - 5.3921089 \times 10^{-6}T^2 + 0.9663917 \times 10^{-9}T^3$$

$$CO_2, S = 41.78458 + 2.0871316 \times 10^{-2}T - 0.6347125 \times 10^{-5}T^2 + 0.9526361 \times 10^{-9}T^3$$

$$Ne, S = 29.5537807 + 1.2917042 \times 10^{-2}T - 5.3907410 \times 10^{-6}T^2 + 0.9659557 \times 10^{-9}T^3$$

3. Equations for the Specific Heat at Constant Pressure (BTU/lbm-mole°R)

Temperature Range 900°-1800°R

$$N_2, C_p = 7.23667810 - 1.3015396 \times 10^{-3}T + 1.5759008 \times 10^{-6}T^2 - 0.3746857 \times 10^{-9}T^3$$

$$O_2, C_p = 5.7846285 + 2.2415270 \times 10^{-3}T - 0.4580023 \times 10^{-6}T^2$$

$$A, C_p = 4.96815$$

$$CO_2, C_p = 5.3131429 + 0.8363827 \times 10^{-2}T - 0.3088999 \times 10^{-5}T^2 + 0.4493104 \times 10^{-9}T^3$$

$$Ne, C_p = 4.96815$$

Table 3. Equations for the Second Virial Coefficient and the Derivatives for the Constituents of Air

1. Nitrogen (N₂)

$$B = \frac{5.1364637 \times 10^2 - 0.6636122T - 0.3534783 \times 10^{-3}T^2}{1.0 - 1.7158299 \times 10^{-2}T - 0.9296798 \times 10^{-5}T^2}$$

$$T \frac{dB}{dT} = \frac{-3.4560792 \times 10^2}{1.0 - 1.1286423 \times 10^{-2}T - 0.29627746 \times 10^{-5}T^2}$$

$$T^2 \frac{d^2B}{dT^2} = \frac{6.7503388 \times 10^2}{1.0 - 0.8951382 \times 10^{-2}T - 0.4815325 \times 10^{-5}T^2 + 1.3834608 \times 10^{-9}T^3}$$

2. Oxygen (O₂)

$$B = \frac{4.2857084 \times 10^2 - 4.7667818 \times 10^{-1}T - 1.5050447 \times 10^{-4}T^2}{1.0 - 1.4123010 \times 10^{-2}T - 0.5095962 \times 10^{-5}T^2}$$

$$T \frac{dB}{dT} = \frac{-3.1691728 \times 10^2}{1.0 - 0.9521198 \times 10^{-2}T - 0.3228332 \times 10^{-5}T^2 + 0.4514126 \times 10^{-9}T^3}$$

$$T^2 \frac{d^2B}{dT^2} = \frac{-3.3796998 \times 10^1 - 4.9627303T + 1.0935667 \times 10^{-2}T^2}{1.0 - 1.9686162 \times 10^{-2}T + 1.2893683 \times 10^{-4}T^2}$$

$$\frac{-0.5888087 \times 10^{-5}T^3 + 0.3089713 \times 10^{-9}T^4}{-0.2105136 \times 10^{-6}T^3 + 0.946670 \times 10^{-10}T^4}$$

3. Argon (A)

$$B = \frac{3.8904656 \times 10^2 - 0.870535T + 0.4772262 \times 10^{-3}T^2 - 1.4860291 \times 10^{-6}T^3}{1.0 - 1.4845725 \times 10^{-2}T + 1.1790085 \times 10^{-5}T^2 + 1.4973286 \times 10^{-10}T^3}$$

$$T \frac{dB}{dT} = \frac{-2.7524532 \times 10^2 + 4.4273617 \times 10^{-2}T}{1.0 - 0.9485511 \times 10^{-2}T}$$

$$T^2 \frac{d^2B}{dT^2} = \frac{3.9858659 \times 10^2 - 3.4251675 \times 10^{-2}T}{1.0 + 0.6811836 \times 10^{-2}T}$$

4. Carbon Dioxide (CO₂)

$$B = \frac{5.3152906 \times 10^2 - 5.0336843 \times 10^{-1}T + 0.7026469 \times 10^{-4}T^2}{1.0 - 0.6113584 \times 10^{-2}T - 2.2018674 \times 10^{-8}T^2}$$

$$T \frac{dB}{dT} = \frac{(1) \quad 5.3458176T - 0.9807759 \times 10^{-3}T^2 - 7.8788948 \times 10^{-9}T^3 + 18.9162693 \times 10^{-12}T^3}{(1.0 - 0.6113584 \times 10^{-2}T - 2.2018674 \times 10^{-8}T^2)}$$

$$T^2 \frac{d^2B}{dT^2} = \frac{(1) \quad 11.8074171T^2 - 125.9326564 \times 10^{-5}T^3 - 1.4462917 \times 10^{-7}T^4 - 47.4547667 \times 10^{-13}T^5 - 50.1159356 \times 10^{-17}T^4}{(1.0 - 1.104452 \times 10^{-2}T - 7.13405040 \times 10^{-8}T^2)^4}$$

5. Neon (Ne)

$$B = \frac{59.425695 - 0.27144987T}{1.0 - 1.646348 \times 10^{-2}T}$$

$$T \frac{dB}{dT} = \frac{-6.1992870 \times 10^1 + 1.8886040 \times 10^{-2}T}{1.0 - 1.7014989 \times 10^{-2}T}$$

$$T^2 \frac{d^2B}{dT^2} = \frac{1.5852079 \times 10^2 - 3.1378493 \times 10^{-2}T}{1.0 - 1.8918656 \times 10^{-2}T}$$

(1) Derivative taken from fitted value of "B".

Table 4. Equations for the Third Virial Coefficients and the Derivatives for the Constituents of Air

1. Nitrogen (N_2)

$$C = \frac{355.28210 - 4.7253632T}{1.0 - 4.7446815 \times 10^{-3} T}$$

$$T \frac{dC}{dT}^{(1)} = \frac{-30.396628 \times 10^{-1} T}{1.0 - 9.4893630 \times 10^{-3} T + 22.5120025 \times 10^{-6} T^2}$$

$$T^2 \frac{d^2C}{dT^2}^{(1)} = \frac{-28.8444637 \times 10^{-3} T^2 + 136.8577931 \times 10^{-6} T^3}{(1.0 - 9.4893630 \times 10^{-3} T + 22.5120025 \times 10^{-6} T^2)^2}$$

2. Oxygen (O_2)

$$C = \frac{-4.2345758 \times 10^3}{1.0 - 0.9728086 \times 10^{-2} T}$$

$$T \frac{dC}{dT}^{(1)} = \frac{4.1194317 \times 10^{-1} T}{1.0 - 0.9728086 \times 10^{-2} T}$$

$$T^2 \frac{d^2C}{dT^2}^{(1)} = \frac{-4.0074185 \times 10^{-3} T^2}{1.0 - 0.9728086 \times 10^{-2} T}$$

3. Argon (A)

$$C = 5.987.9538 - 19.016416T + 2.4336141 \times 10^{-2} T^2 - 1.0787834 \times 10^{-5} T^3$$

$$T \frac{dC}{dT}^{(1)} = -19.016416T + 486.72282 \times 10^{-4} T - 3.2363502 \times 10^{-5} T^3$$

$$T^2 \frac{d^2C}{dT^2}^{(1)} = 486.72282 \times 10^{-4} T^2 - 6.4727004 \times 10^{-5} T^3$$

4. Carbon Dioxide (CO_2)

$$C = 11517.385 - 13.38398T + 0.3190838 \times 10^{-2} T^2$$

$$T \frac{dC}{dT}^{(1)} = -13.38398T + 0.6381676 \times 10^{-2} T^2$$

$$T^2 \frac{d^2C}{dT^2}^{(1)} = 0.6381676 \times 10^{-2} T^2$$

5. Neon (Ne)

$$C = 0.0$$

$$T \frac{dC}{dT} = 0.0$$

$$T^2 \frac{d^2C}{dT^2} = 0.0$$

(1) Derivative taken from fitted value of C.

Table 5. Equations for the Thermodynamic Properties for the Constituents of the Exhaust Gas

1. Equations for Sensible Enthalpy (BTU/lbm-mole)

Temperature Range -900°-1800°R

$$\text{N}_2, H = 272.57872 + 6.2849888T + 4.2460662 \times 10^{-4}T^2$$

$$\text{O}_2, H = -49.9253121 + 6.8005911T + 4.6097941 \times 10^{-4}T^2$$

$$\text{A}, H = 0.19368 + 4.9682152T$$

$$\text{CO}_2, H = -291.6316413 + 6.5377190T + 28.320187 \times 10^{-4}T^2 - 0.3858033 \times 10^{-6}T^3$$

$$\text{Ne}, H = 0.19368 + 4.9682152T$$

$$\text{H}_2\text{O}, H = 356.6510897 + 6.913576T + 8.1349063 \times 10^{-4}T^2$$

Temperature Range - 1800°R-2700°R

$$\text{N}_2, H = -220.5134204 + 6.8101302T + 2.8505033 \times 10^{-4}T^2$$

$$\text{O}_2, H = -630.6330969 + 7.3851082T + 2.599229 \times 10^{-4}T^2$$

$$\text{A}, H = -0.0615 + 4.9681418T$$

$$\text{CO}_2, H = -3294.0760689 + 11.07844T + 5.4166925 \times 10^{-4}T^2$$

$$\text{Ne}, H = -0.0615 + 4.9681418T$$

$$\text{H}_2\text{O}, H = 152.8596437 + 7.1089372T + 7.6785528 \times 10^{-4}T^2$$

Temperature Range -2700°-4000°R

$$\text{N}_2, H = -1304.1576077 + 7.6123722T + 1.3657170 \times 10^{-4}T^2$$

$$\text{O}_2, H = 1204.9978428 + 7.8839888T + 1.5887864 \times 10^{-4}T^2$$

$$\text{A}, H = -0.02187 + 4.9681271T$$

$$\text{CO}_2, H = -5537.3281389 + 12.747913T + 2.3106225 \times 10^{-4}T^2$$

$$\text{Ne}, H = -0.02187 + 4.9681271T$$

$$\text{H}_2\text{O}, H = 1858.4935816 + 8.5657282T + 5.0420885 \times 10^{-4}T^2$$

2. Equations for Chemical plus Sensible Enthalpy (BTU/lbm-mole)

Temperature Range 1800°-2700°R

$$\text{N}_2, H = -20.5134204 + 6.8101302T + 2.8505033 \times 10^{-4}T^2$$

$$\text{O}_2, H = -630.6330969 + 7.3851082T + 2.5992293 \times 10^{-4}T^2$$

$$\text{A}, H = -0.0615 + 4.9682152T$$

$$\text{CO}_2, H = -175045.8247470 + 13.506027T$$

$$\text{Ne}, H = -0.0615 + 4.9682152T$$

$$\text{H}_2\text{O}, H = -102632.3476190 + 7.1088046T + 7.678847 \times 10^{-4}T^2$$

Table 5. Continued

Temperature Range - 2700°-4000°R

$$N_2, H = -1304.1576077 + 7.6123722T + 1.3657170 \times 10^{-4}T^2$$

$$O_2, H = -1240.9978428 + 7.8839888T + 1.5887864 \times 10^{-4}T^2$$

$$A, H = -0.02187 + 4.9681271T$$

$$CO_2, H = -177175.4038470 + 14.294766T$$

$$Ne, H = -0.02187 + 4.9681271T$$

$$H_2O, H = -104643.9857996 + 8.5658373T + 5.0418784 \times 10^{-4}T^2$$

Temperature Range: 2000°-4000°R

$$H, H = 9.2937814 \times 10^4 + 4.9679289T$$

$$O, H = 1.0650436 \times 10^5 + 4.9819292T$$

$$OH, H = 1.7243891 \times 10^4 + 6.5117725T + 2.4740577 \times 10^{-4}T^2$$

$$NO, H = 3.7810593 \times 10^4 + 7.7703187T + 1.3914575 \times 10^{-4}T^2$$

$$CO, H = 4.9950257 \times 10^4 + 7.4991057T + 1.6384251 \times 10^{-4}T^2$$

$$H_2, H = 4.379566 \times 10^2 + 6.2305090T + 2.7323736 \times 10^{-4}T^2$$

3. Equations for Entropy (less - $RLnp_i$ term), (BTU/lbm-mole, °R)

Temperature Range 900-1800°R

$$N_2, S = 39.251394 + 0.0155587T - 0.5615997 \times 10^{-5}T^2 + 0.933764 \times 10^{-9}T^3$$

$$O_2, S = 42.269726 + 1.5770590 \times 10^{-2}T - 0.5390427 \times 10^{-5}T^2 + 0.8573795 \times 10^{-9}T^3$$

$$A, S = 31.5883510 + 1.2918283 \times 10^{-2}T - 5.3921089 \times 10^{-6}T^2 + 0.9663917 \times 10^{-9}T^3$$

$$CO_2, S = 41.78458 + 2.0871316 \times 10^{-2}T - 0.6347125 \times 10^{-5}T^2 + 0.9526361 \times 10^{-9}T^3$$

$$Ne, S = 29.5537807 + 1.2917042 \times 10^{-2}T - 5.3907410 \times 10^{-6}T^2 + 0.9659557 \times 10^{-9}T^3$$

$$H_2O, S = 37.437166 + 1.8092773 \times 10^{-2}T - 0.6382909 \times 10^{-5}T^2 + 1.0748317 \times 10^{-9}T^3$$

Temperature Range - 1800°-2700°R

$$N_2, S = 57.275024 - 1.8300467 \times 10^{-2}T + 1.7559820 \times 10^{-5}T^2 - 0.5815832 \times 10^{-8}T^3$$

$$O_2, S = 47.225630 + 0.7577402 \times 10^{-2}T - 0.828194 \times 10^{-6}T^2$$

$$A, S = 36.4464480 - 4.5571014 \times 10^{-3}T - 0.5119033 \times 10^{-6}T^2$$

$$CO_2, S = 47.518398 - 1.1512786 \times 10^{-2}T - 1.2066643 \times 10^{-6}T^2$$

$$Ne, S = 34.4116312 + 4.5570565 \times 10^{-3}T - 0.5118049 \times 10^{-6}T^2$$

$$H_2O, S = 43.261707 + 0.8244883 \times 10^{-2}T - 0.7782285 \times 10^{-6}T^2$$

Table 5. Continued

Temperature Range - 2700°-4000°R

$$N_2, S = 46.8564740 + 5.0506990 \times 10^{-3} T - 0.3700634 \times 10^{-6} T^2$$

$$O_2, S = 50.2049115 + 5.2780447 \times 10^{-3} T - 0.3852719 \times 10^{-6} T^2$$

$$A, S = 38.5124276 + 3.0262745 \times 10^{-3} T - 0.22832958 \times 10^{-6} T^2$$

$$CO_2, S = 51.5035705 + 8.44472 \times 10^{-3} T - 0.6170116 \times 10^{-6} T^2$$

$$Ne, S = 34.8197332 + 4.5503522 \times 10^{-3} T - 0.6902733 \times 10^{-6} T^2 + 0.0462520 \times 10^{-9} T^3$$

$$H_2O, S = 45.6963147 + 0.6353274 \times 10^{-2} T - 0.4115987 \times 10^{-6} T^2$$

4. Equations for the Specific Heat at Constant Pressure (BTU/lbm-mole°R)

Temperature Range - 900°-1800°R

$$N_2, C_p = 7.23667810 - 1.3015396 \times 10^{-3} T + 1.5759008 \times 10^{-6} T^2 - 0.3746857 \times 10^{-9} T^3$$

$$O_2, C_p = 5.7846285 + 2.2415270 \times 10^{-3} T - 0.4580023 \times 10^{-6} T^2$$

$$A, C_p = 4.96815$$

$$CO_2, C_p = 5.3131429 + 0.8363827 \times 10^{-2} T - 0.3088999 \times 10^{-5} T^2 + 0.4493104 \times 10^{-9} T^3$$

$$Ne, C_p = 4.96815$$

$$H_2O, C_p = 7.5482768 + 4.2815697 \times 10^{-4} T + 0.7157717 \times 10^{-6} T^2 - 1.3495489 \times 10^{-10} T^3$$

Temperature Range 1800°-2700°R

$$N_2, C_p = 5.7766562 + 1.5061552 \times 10^{-3} T - 0.8888113 \times 10^{-6} T^2 + 1.0954859 \times 10^{-10} T^3$$

$$A, C_p = 4.96815$$

$$CO_2, C_p = 6.680396 + 0.5990060 \times 10^{-2} T - 1.7096379 \times 10^{-6} T^2 + 0.1809910 \times 10^{-9} T^3$$

$$Ne, C_p = 4.96815$$

$$H_2O, C_p = 7.1564387 + 0.9855705 \times 10^{-3} T + 0.4640690 \times 10^{-6} T^2 - 1.0002320 \times 10^{-10} T^3$$

Temperature Range - 2700° 4000°R

$$N_2, C_p = 6.5727317 + 0.9099083 \times 10^{-3} T - 0.9596494 \times 10^{-7} T^2$$

$$O_2, C_p = 7.6813079 + 4.4281245 \times 10^{-4} T - 1.8738208 \times 10^{-8} T^3$$

$$A, C_p = 4.96815$$

$$CO_2, C_p = 10.8521173 + 1.6107530 \times 10^{-3} T - 1.7125528 \times 10^{-7} T^2$$

$$Ne, C_p = 4.96815$$

$$H_2O, C_p = 5.9764766 + 2.5861179 \times 10^{-3} T - 2.3692669 \times 10^{-7} T^2$$

Table 5. Concluded

5. Equations for the Gibbs Free Energy Function (BTU/lbm-mole)

Temperature Range - 2000°R-4000°R

$$\begin{aligned}
 \text{H, } F^\circ &= 5.3150524 \times 10^4 - 15.6253583 T - 0.9767035 \times 10^{-3} \times 10^{-3} T^2 + 0.5610564 \times 10^{-7} T^3 \\
 \text{O, } F^\circ &= 6.0670223 \times 10^4 - 21.8518477 T - 0.9782325 \times 10^{-3} T^2 + 0.5614114 \times 10^{-7} T^3 \\
 \text{OH, } F^\circ &= 1.0843812 \times 10^4 - 24.8213338 T - 1.4149044 \times 10^{-3} T^2 + 0.7304718 \times 10^{-7} T^3 \\
 \text{NO, } F^\circ &= 2.2896290 \times 10^4 - 28.1298227 T - 1.5979361 \times 10^{-3} T^2 + 0.8680263 \times 10^{-7} T^3 \\
 \text{CO, } F^\circ &= 2.5226419 \times 10^4 - 26.3634922 T - 1.5649177 \times 10^{-3} T^2 + 0.8457005 \times 10^{-7} T^3 \\
 \text{H}_2, F^\circ &= 1.4415362 \times 10^3 - 17.8897838 T - 1.3549595 \times 10^{-3} T^2 + 0.6781319 \times 10^{-7} T^3 \\
 \text{N}_2, F^\circ &= 1.2087000 \times 10^3 - 25.6082461 T - 1.5325905 \times 10^{-3} T^2 + 0.8179650 \times 10^{-7} T^3 \\
 \text{O}_2, F^\circ &= 1.2814893 \times 10^3 - 27.3792772 T - 1.6271943 \times 10^{-3} T^2 + 0.8783605 \times 10^{-7} T^3 \\
 \text{CO}_2, F^\circ &= -9.2608408 \times 10^4 - 27.9578811 T - 2.5501816 \times 10^{-3} T^2 + 1.3506145 \times 10^{-7} T^3 \\
 \text{H}_2\text{O, } F^\circ &= 5.6574736 \times 10^4 - 25.0072600 T - 1.8841889 \times 10^{-3} T^2 + 0.8839907 \times 10^{-7} T^3
 \end{aligned}$$

APPENDIX A INFLUENCE OF CHEMICAL MODEL ON AFTERBURNER EFFICIENCY CALCULATIONS

In recent years, there has been some variations in the chemical model used to determine turbine engine performance for the case of low efficiencies in afterburner tests. A comparison of several chemical models was made to determine the differences in the calculated afterburner efficiency. Four models were investigated as follows:

1. No effects of chemical dissociation, but with prescribed proportions of CO,
2. No effects of chemical dissociation, but with prescribed quantities of unburned fuel in the exhaust,
3. Complete chemical equilibrium, and
4. Complete chemical equilibrium, but with prescribed quantities of unburned fuel in the exhaust.

Calculations were carried out with the models modified to include observed (Refs. 26 to 29) high levels of carbon monoxide (CO) and unburned fuel (as CH₂ in the model). In the limit, either of these species can represent the effects of less than ideal combustion efficiency. The computer model was basically a real gas Rayleigh line heat addition model with exhaust conditions and composition defined by the program of Ref. 18.

Model (1) was chosen to provide the baseline calculations. The calculated inlet conditions for the afterburner are listed in Table A-1. It was assumed that the inlet fuel/air ratio would be increased to 0.06 in the afterburner. The inlet temperature and pressure were assumed to be 1,300°R and 0.5 atm, respectively, and the inlet Mach number was 0.2.

Calculations were carried out assuming that a prescribed proportion of the theoretical CO₂ (without CO in the exhaust) is converted to CO. The calculated nozzle exhaust total pressures and temperatures together with the combustion efficiency are shown in Table A-2. The efficiency was evaluated as follows:

$$\eta = \left[(h_{o_{ex}} - h_{o_{in}}) \left(\frac{1 + f_{in}}{1 + f_{ex}} \right) \right] \frac{(1 + f_{ex})}{(t_{ex} - t_{in}) \Delta h_f}$$

where h_o denotes sensible total enthalpy, f denotes fuel/air ratio, Δh_f , the lower heating value of fuel, and subscripts in and ex denote afterburner inlet and nozzle exhaust conditions, respectively. The sensible enthalpy was evaluated by subtracting the static enthalpy (sensible plus chemical) at 298.15°K from the total enthalpy, mixture composition being the same for both enthalpy calculations.

Having determined the exhaust conditions for model (1), the sensible enthalpy changes and efficiency were evaluated with models (2) through (4), assuming the same nozzle exhaust total temperature obtained with model (1). The chemical equilibrium was modified to include unburned fuel as a species.

The calculated afterburner efficiencies for the four models are shown in Table A-3, and the concentrations of CO and unburned fuel used in the calculations are shown in Table A-4. The efficiencies in Table A-3 show no significant difference for a given set of conditions regardless of the calculation model used. This means that the calculated enthalpies for the various models are essentially the same, and therefore, the choice of models is not important over the range of these calculations.

The ratio of efficiencies for the different models is so close, even at the 3,246°R temperature, that it should be possible to increase the base temperature below which assuming no dissociation should be an adequate model. This could result in a significant reduction in data manipulation time with on-line data acquisition systems.

Table A-1. Afterburner Inlet Conditions

<u>Parameter</u>	<u>Total Conditions</u>	<u>Static Conditions</u>
Pressure	0.5 atm	0.4868 atm
Temperature	1300°R	1291.1°R
Specific Heat	0.267 Btu/lb°R	0.267 Btu/lb°R
Ratio of Specific Heats	1.346	1.346
Entropy	1.9625 Btu/lb°R	1.9625 Btu/lb°R
Speed of Sound	1733.3 ft/sec	1727.1 ft/sec
Mach Number	0	0.2
Density	0.01525 lb/ft ³	0.01495 lb/ft ³
Molecular Weight	28.956 lb/lb-mole	28.956 lb/lb-mole
Fuel-to-Air Ratio	0.025 lb _{fuel} /lb _{air}	

Table A-2. Nozzle Exhaust Total Conditions with Prescribed CO Concentrations

	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1
CO_2/CO_2_{max}										
Total Pressure	0.4875	0.4867	0.486	0.4852	0.4845	0.4838	0.483	0.4823	0.4816	0.4809
Total Temperature	2566.6	2643.8	2720.5	2796.8	2872.7	2948.1	3023.2	3097.8	3172.1	3246.1
Specific Heat	0.3086	0.3104	0.3122	0.3139	0.3156	0.3173	0.3188	0.3204	0.3218	0.3233
Ratio of Specific Heat	1.2959	1.2926	1.2893	1.2862	1.2832	1.2803	1.2775	1.2748	1.2722	1.2696
Entropy	2.2274	2.2319	2.236	2.2397	2.2432	2.2462	2.2489	2.2512	2.2531	2.2542
Speed of Sound	2261.9	2291.0	2319.4	2347.0	2373.9	2400.2	2425.8	2450.8	2475.2	2499.1
Mach Number	1	1	1	1	1	1	1	1	1	1
Density	0.004591	0.004462	0.00434	0.004227	0.00412	0.004019	0.003924	0.003824	0.003748	0.003667
Molecular Weight	28.202	28.283	28.364	28.446	28.528	28.611	28.694	28.778	28.862	28.946
Efficiency	0.639	0.679	0.719	0.759	0.799	0.839	0.879	0.919	0.959	1

Data: Inlet sensible enthalpy $h_{o_{in}} = 194.8$ Btu/lbLower heat of combustion $\Delta h_f = 18,650$ Btu/lb $CO_2_{max} = 11.724$ percent

Table A-3. Afterburner Efficiencies

$P_{O_{ex}}$	$T_{O_{ex}}$	η_1	η_2 & η_4	η_3	η_1/η_3	η_2/η_3
0.4875	2567	0.639	0.647	0.643	0.994	1.006
0.4867	2644	0.679	0.688	0.683	0.994	1.007
0.486	2720	0.719	0.729	0.723	0.995	1.008
0.4852	2797	0.759	0.768	0.763	0.995	1.008
0.4845	2873	0.799	0.808	0.803	0.995	1.006
0.4838	2948	0.839	0.846	0.843	0.995	1.004
0.483	3023	0.879	0.886	0.882	0.996	1.004
0.4823	3098	0.919	0.925	0.922	0.997	1.003
0.4816	3172	0.959	0.964	0.962	0.997	1.002
0.4809	3246	1.000	1.000	1.000	1.000	1.000

Table A-4. CO and Fuel Vapor Exhaust Concentrations

$T_{O_{ex}}$	1 % CO	2 ppmv CO	3 ppmv CO	4 & Fuel
2567	5.14	1.0	1.7	1.56
2644	4.58	2.3	3.4	1.38
2720	4.02	4.0	6.4	1.2
2797	3.46	10.0	11.8	1.02
2873	2.89	19.0	21.0	0.85
2948	2.32	32.0	36.1	0.68
3023	1.74	50.0	60.3	0.51
3098	1.17	82.0	97.8	0.34
3172	0.584	130.0	154.7	0.17
3246	0	239.2	239.2	0

APPENDIX B
COMPUTER PROGRAM LISTINGS

FORTRAN IV G LEVEL 21

MAIN

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```

      C MAIN PROGRAM
0001 REAL M,MW,AIR
0002 READ(5,10)LP,NP
0003 10 FORMAT(12,2X,12)
0004 ITEM = 0
0005 16 WRITE(LP,4)
0006 4 FORMAT(1H1)
0007 WRITE(LP,5)
0008 5 FORMAT(1H,35HTHERMOODYNAMIC PROPERTIES - CHECKOUT//120H TEMPERATUR
      1E PRESSURE HEAT. VALUE FUEL/AIR ENTHALPY ENTROPY SPE
      2CIFIC HEAT WTM CASE /)
0009 15 CONTINUE
0010 READ(NP,20)TEMP1,PRES1,HEATV1,FAIR1,M1,XKON1
0011 20 FORMAT(6E10.0)
0012 TEMP = TEMP1
0013 IF(TEMP)50,50,10
0014 18 CONTINUE
0015 PRES = PRES1
0016 HEATV = HEATV1
0017 FAIR = FAIR1
0018 M = M1
0019 XKON = XKON1
0020 ITEM = ITEM+1
0021 CALL THERMO(TEMP,PRES,HEATV,FAIR,XKON,M,S,CP,WTM,LP,ITEM)
0022 WRITE(LP,30)TEMP,PRES,HEATV,FAIR,M,S,CP,WTM,ITEM
0023 30 FORMAT(1H,4F12.4,2F12.5,3X,2F12.5,5X,14)
0024 45 CONTINUE
0025 GO TO 15
0026 50 CONTINUE
0027 STOP
0028 END

```

FORTRAN IV G LEVEL 21

THERMO

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```

0001      SUBROUTINE THERMO(TR,P,MV,F,XKON,MH,SS,CPP,WTM,LP,ITEM)
0002      REAL M,MWAIR
0003      COMMON/CATHY/XN2,XO2,XAR,XCO2,XNE,MWAIR,Y(I4),X(I10),PAR,PNE
0004      PA = P/14.696
0005      C      MOLE FRACTIONS OF CONSTITUENTS OF AIR
0006      XN2 = 0.78084
0007      XO2 = 0.209476
0008      XAR = 0.00934
0009      XCO2 = 0.0003194
0010      XNE = 0.0000246
0011      C      MOLECULAR WEIGHT OF CONSTITUENTS
0012      C      1-N2,2-O2,3-AR,4-CO2,5-NE,6-H2O,7-H,8-O,9-OH,10-NO,11-CO,12-H2,13-C,14-N
0013      Y(1) = 28.0134
0014      Y(2) = 31.9988
0015      Y(3) = 39.944
0016      Y(4) = 44.00995
0017      Y(5) = 20.183
0018      Y(6) = 18.016
0019      Y(7) = 1.00797
0020      Y(8) = 16.0
0021      Y(9) = 17.0074
0022      Y(10) = 30.0008
0023      Y(11) = 28.01055
0024      Y(12) = 2.016
0025      Y(13) = 12.011
0026      Y(14) = 14.008
0027      C      MOLECULAR WEIGHT OF AIR
0028      MWAIR = 28.9646
0029      C      HYDROGEN/CARBON ATOM RATIO
0030      M=0.1636
0031      R = 1.987165 * 778.28
0032      RA = R/MWAIR
0033      RB = (RA * ((F * R * M)/(2.*Y(12)* (1.0 * M)))) / (1.0 * F)
0034      XHWGAS = R/RB
0035      WTM = XHWGAS
0036      C      CHECK FOR ENTHALPY KNOWN CASE TO CALCULATE TEMPERATURE
0037      IF(MH)10002,10000,10001
0038      I0001 TI=3000.*182.*ALOG10(PA)
0039      HI=0
0040      SS=0
0041      CPP=0
0042      CALL GAS(TI,PA,HI,SS,CPP,F,M,LP,ITEM)
0043      C      EXHAUST GAS-CHECK FOR DISSOCIATION OR NON-DISSOCIATION
0044      IF(HI-MH)10002,10004,10003
0045      I0004 TR = TI
0046      RETURN
0047      I0003 CALL GAS(TR,PA,MH,SS,CPP,F,M,LP,ITEM)
0048      RETURN
0049      I0002 ICON=1.0
0050      TR = 3000.0
0051      CALL CHEMEO(PA,TR,F,MV,ICON,XKON,MH,SS,CPP,WTM,LP,ITEM)
0052      RETURN
0053      C      CHECK FOR AIR OR EXHAUST GAS
0054      I0000 IF(F)51,100,50
0055      50 TI = 3000.0 * 182. * ALOG10(PA)
0056      IF(TR.GT.TI)GO TO 59

```

FORTRAN IV G LEVEL 2I

THERMO

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```

0049      CALL GAS(TR,PA,MM,SS,CPP,F,M,LP,ITEM)
0050      RETURN
          C      TI=5000.0
0051      59 CONTINUE
0052      ICON = I
0053      MR=0.0
0054      MG=0
0055      CALL CHEMEQ(PA,TR,F,MV,ICON,XKON,MM,SS,CPP,WTM,LP,ITEM)
0056      CALL CHEMEQ(PA,TI,F,MV,ICON,XKON,MR,SR,CPR,WTR,LP,ITEM)
0057      CALL GAS(TI,PA,MG,SG,CPG,F,M,LP,ITEM)
0058      DELM = MM - MR
0059      MM = MG + DELM
0060      DELCP = CPP - CPR
0061      CPP = CPG + DELCP
0062      DELS = SS - SR
0063      SS = SG + DELS
0064      RETURN
          C      AIR EQUATIONS
0065      100 CALL GAS(TR,PA,MM,SS,CPP,F,M,LP,ITEM)
          C      WTM = MWAIR
          RETURN
0066      51 WRITE(LP,52) ITEM,F
0067      52 FORMAT(1H ,I4,2X,6MTHERMO,2X,15MINCORRECT INPUT,3X,3HF =,F12.4)
0068      RETURN
0069      END
0070

```

FORTRAN IV G LEVEL 21

GAS

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```

0001      SUBROUTINE GAS(TR,PA,HB,SB,CPB,F,M,LP,ITEM)
0002      REAL M,MWAIR
0003      DATA CTR2/0.0/
0004      COMMON/CATHY/XN2,XO2,XAR,XCO2,XNE,MWAIR,Y(14),CHASCO(10),PAR,PNE
0005      DIMENSION H(6),S(6),CP(6),C1(4),C2(4),C3(4),H1(72),S1(72),CP1(72),
1X(6)
0006      X(1) = XN2
0007      X(2) = XO2
0008      X(3) = XAR
0009      X(4) = XCO2
0010      X(5) = XNE
0011      X(6) = 0.0
0012      HIG=0.0
0013      HC=0.0
0014      IF(F.EQ.0.)HB=0.0
0015      IF(F.EQ.0.)GO TO 74
0016      CALL MFNOD(X(1),F)
0017      IF(HB.GT.100.0)GOTO72
0018      IF(HB.EQ.-1.0)GO TO 72
0019      74 IF(TR-4000.0)75,300,999
0020      75 IF(TR-300.0)999,200,76
0021      76 IF(TR-900.0)200,300,300
C      AIR PROPERTIES 300R.-900R.
0022      200 CALL HSCP(TR,1,1,H(1))
0023      CALL HSCP(TR,1,2,S(1))
0024      CP(1) = (((-0.4421008E-12 *TR) + 1.5962495E-09)*TR -
1      1.356283E-06) * TR + 4.1982143E-04) * TR +
2      6.9153738
0025      CALL HSCP(TR,2,1,H(2))
0026      CALL HSCP(TR,2,2,S(2))
0027      CALL HSCP(TR,2,3,CP(2))
0028      H(3) = 4.96815*TR
0029      S(3) = 4.96815 * ALOG(TR/1.8) + 8.6765909
0030      CP(3) = 4.96815
0031      CALL HSCP(TR,4,1,H(4))
0032      CALL HSCP(TR,4,2,S(4))
0033      CALL HSCP(TR,4,3,CP(4))
0034      H(5) = 4.96815 * TR
0035      S(5) = 4.96815 * ALOG(TR/1.8) + 6.6417222
0036      CP(5) = 4.96815
0037      CALL HSCP(TR,5,1,H(6))
0038      CALL HSCP(TR,5,2,S(6))
0039      CALL HSCP(TR,5,3,CP(6))
0040      DO 6 I=1,6
0041      IF(X(I).LE.0.)GO TO 5
0042      S(I) = S(I) -1.987165 * ALOG(X(I). * PA)
0043      GO TO 6
0044      5 S(I) = 0.
0045      6 CONTINUE
0046      GO TO 1000
C      AIR AND REVISED PROPERTIES 900R-4000R
0047      72 HC=0
0048      HC=HB
0049      TR = 250.
0050      IF(HC):04,104,300
0051      300 CALL CLEFF(7,H1)

```

FORTRAN IV G LEVEL 21

GAS

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0052      CALL COEFF(8,S1)
0053      CALL COEFF(9,CP1)
0054      IF (TR .LE. 4000.0) KA=48
0055      IF (TR .LE. 2700.0) KA=24
0056      IF (TR.LE.1800.)KA=0
0057      DO 400 K=1,6
0058      H(K) = 0.0
0059      S(K) = 0.0
0060      CP(K) = 0.0
0061      KK = 4 * (K-1) * KA
0062      DO 500 J=1,4
0063      KKK = KK * J
0064      TX = TR ** (J-1)
0065      C1(J) = H1(KKK) * TX
0066      C2(J) = S1(KKK) * TX
0067      C3(J) = CP1(KKK) * TX
0068      DO 30 J=1,4
0069      H(K) = H(K) + C1(J)
0070      S(K) = S(K) + C2(J)
0071      CP(K) = CP(K) + C3(J)
0072      IF (K-1) 320,315,320
0073      315 IF (TR .LE. 2700.0, AND. TR .GT. 1800.0) S(K) = S(K) * 0.6848142E-12
0074      320 CONTINUE
0075      400 CONTINUE
0076      DO 15 I=1,6
0077      IF (X(I).LE.0.) GO TO 14
0078      S(I) = S(I) - 1.987165 * ALOG(X(I) * PA)
0079      GO TO 15
0080      14 S(I) = 0.
0081      15 CONTINUE
0082      1000 HA = XN2 * H(1) * XO2 * H(2) * XAR * H(3) * XCO2 * H(4) * XNE * H(5)
0083      HAIR = HA / MWAIR
0084      C CALCULATION OF PROPERTIES-AEDC-TR-75- -SECT.2.2.1
0085      AH = (H(6) - .5 * H(2)) / Y(12)
0086      BH = (H(4) - H(2)) / Y(13)
0087      Z = 1. / (1. * F)
0088      MB = Z * (HAIR * F * (AH * M + BH) / (1. * M))
0089      SA = XN2 * S(1) * XO2 * S(2) * XAR * S(3) * XCO2 * S(4) * XNE * S(5)
0090      SAIR = SA / MWAIR
0091      AE = (S(6) - .5 * S(2)) / Y(12)
0092      BE = (S(4) - S(2)) / Y(13)
0093      SB = Z * (SAIR * F * (AE * M + BE) / (1. * M))
0094      CPA = XN2 * CP(1) * XO2 * CP(2) * XAR * CP(3) * XCO2 * CP(4) * XNE * CP(5)
0095      CPAIR = CPA / MWAIR
0096      AC = (CP(6) - .5 * CP(2)) / Y(12)
0097      BC = (CP(4) - CP(2)) / Y(13)
0098      CPB = (CPAIR * F * (AC * M + BC) / (M * 1.)) / (1. * F)
0099      71 IF (MC .GT. 1.E-6) GO TO 73
0100      73 DELT = (MC - MB) / CPB
0101      IF (ABS(DELT) .LE. 0.001 * TR) GO TO 105
0102      CTR2 = CTR2 + 1.0
0103      IF (CTR2 .GT. 25.0) GO TO 105
0104      IF (DELT) 70, 105, 70
0105      70 TR = TR + DELT

```

FORTRAN 1V G LEVEL 21 GAS DATE = 75224 13/41/03

```

0106      GO TO 300
0107      69 TR=TR-OELT
0108      WRITE(6,68)TI,PA,MIG,MC,MB
0109      68 FORMAT(12H GAS =,10E12.6)
0110      GO TO 300
0111      105 RETURN
C          CALCULATION OF AIR PROPERTIES WITH INTERMOLECULAR CORRECTION
C          CALCULATION OF PROPERTIES-AEOC-TR-75- -SECT.2.1.4
0112      150 CPB = CPMIX(PA,TR,CPAIR,LP,ITEM)
0113      MB = MMIX(PA,TR,MAIR,LP,ITEM)
0114      SB = SMIX(PA,TR,SAIR,LP,ITEM)
0115      RETURN
0116      999 WRITE(LP,250)ITEM
0117      250 FORMAT(1H ,14,2X,6HTHERMO,2X,25H TEMPERATURE OUT OF RANGE)
0118      MB = 0.0
0119      SB = 0.0
0120      CPB = 0.0
0121      RETURN
0122      END

```

FORTRAN 1V G LEVEL 21 MFN00 DATE = 75224 13/41/03

```

0001      SUBROUTINE MFN00(X,F)
C          CALCULATION OF EXHAUST GAS COMPOSITION-T,LE,TI,
0002      REAL MWAIR,MN2,MO2,MAR,MCO2,MNE,MM20,MWFL
0003      COMMON/CATHY/XN2,XO2,XAR,XCO2,XNE,MWAIR,Y(14),Z(10),PAR,PNE
0004      DIMENSION X(6)
0005      XN = 1.0
0006      XM=1.95
0007      MWFL = 12.011 * XN + 1.00797 * XM
0008      FAM = F * MWAIR/MWFL
0009      MN2 = XN2/FAM
0010      MO2 = XO2/FAM - XN - XM/4.
0011      MAR = XAR/FAM
0012      MCO2 = XCO2/FAM + XN
0013      MNE = XNE/FAM
0014      MM20 = XM/2.
0015      TM = MN2 + MO2 + MAR + MCO2 + MNE + MM20
0016      X(1) = MN2/TM
0017      X(2) = MO2/TM
0018      X(3) = MAR/TM
0019      X(4) = MCO2/TM
0020      X(5) = MNE/TM
0021      X(6) = MM20/TM
0022      RETURN
0023      END

```

FORTRAN IV G LEVEL 21

CHEMEQ

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```

0001      SUBROUTINE CHEMEQ(PA,T,F,MV,ICON,XKON,H,S,CP,WTM,LP,ITEM)
0002      REAL M
0003      COMMON/CATHY/XN2,XO2,XAR,XCO2,XNE,MWAIR,Y(14),X(10),PAR,PNE
C      THIS SUBROUTINE INITIALIZES THE RHOES AND OSGERBY EQUATIONS
C      TO CALCULATE THE PROPERTIES OF A DISSOCIATED EXHAUST GAS
0004      XN = 1.0
0005      XM = 1.95
0006      XX = 0.209476/(XN + 0.25 * XM)
C      STOICHIOMETRIC RATIO = 0.06795 FOR CNH1.95N
0007      PH1 = F/ 0.06795
0008      C = 2.0 * XO2 + 2.0 * XCO2
0009      D = 2.0 * XN2
0010      E = XAR
0011      G=XNE
0012      A = XCO2 + PH1 * XX
0013      B = PH1 * XX * XM
0014      IF(XKON)10,20,10
0015      10 CALL FUELM(A,B,PH1,XX,XM,MV,M)
0016      GO TO 66
0017      20 CONTINUE
0018      IF(M.GT.0..AND.XKON.EQ.0.)GO TO 30
0019      CALL PROP(A,B,C,D,E,G,T,PA,H,S,CP,WTM,X,PAR,PNE,TM,NT,ICON,LP,
        $ITEM)
0020      RETURN
0021      30 TI=3000.+182.*ALOG10(PA)
0022      M=(XM*Y(7))/(XN*Y(13))
0023      CALL GAS(TI,PA,HIG,SS,CPP,F,M,LP,ITEM)
0024      DELM = M - HIG
0025      HIP=0.0
0026      CALL PROP(A,B,C,D,E,G,TI,PA,HIP,S,CP,WTM,X,PAR,PNE,TM,NT,ICON,
        $LP,ITEM)
0027      M = HIP + DELM
0028      66 ICON=0.0
0029      T=0.0
0030      CALL PROP(A,B,C,D,E,G,T,PA,H,S,CP,WTM,X,PAR,PNE,TM,NT,ICON,
        $LP,ITEM)
0031      RETURN
0032      END

```


FORTRAN IV G LEVEL 21

PROP

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```

0001      SUBROUTINE PROP(CAR,HYD,OX,AN2,AR,ANE,TT,PR,H,S,CP,WTM,P,PAR,PNE,
          *TIME,NT,IT,LP,ITEM)
0002      COMMON/CATMY/XNT,XO2,XAR,XCO2,XNE,MWAIR,Y(I4)
          SPECIES ARE 1-H,2-O,3-OH,4-NO,5-CO,6-H2,7-O2,8-H2O,9-CO2,10-N2,
          C 11-N,12-C,13-N,14-C
          C SUBROUTINE FOR DETERMINING EQUILIBRIUM PARTIAL PRESSURES
          C T IS TEMP. IN DEG R AND CAN BE EITHER INPUT OR OUTPUT
          C P IS PRESS IN ATMOSPHERES AND IS AN INPUT
          C H IS THE ENTHALPY IN BTU PER LBM AND IS EITHER AN INPUT OR OUTPUT
          C S IS THE ENTROPY IN BTU PER LBM-DEG R AND IS AN OUTPUT
          C CP IS THE SPECIFIC HEAT IN BTU PER LBM-DEG R AND IS AN OUTPUT
          C WTM IS THE MOLECULAR WT OF THE MIXTURE AND IS AN OUTPUT
          C NT IS THE NO. OF ITERATIONS TO FIND PARTIAL PRESS AND IS AN OUTPUT
          C IT IS A CONTROL CONSTANT FOR THE SUBROUTINE
          C IT=0 H AND P ARE KNOWN AND T,CP,S, AND WTM ARE FOUND
          C IT=1 T & P ARE KNOWN - H,S,CP,WTM, AND PARTIAL PRESSURES FOUND
0003      DIMENSION O(13),O2(13),O4(13),O5(13),O6(13),O7(13),O8(13),O9(13),O10
          *(3),O3(3),E(6)
0004      DIMENSION DAR(3),ONE(3)
0005      DIMENSION F(12),A1(3),A2(3),A3(3),P(10)
          C CHANGE UNITS OF INPUTS TO BE COMPATIBLE WITH PROGRAM
0006      T = (5./9.)*TT
0007      HO=H
          C
0008      ICT=0
0009      DELT=0.
0010      DO 300 I=1,10
0011      300 P(I)=0.
0012      DELL=.0001
0013      FUEL=2.*CAR+.S*HYD
          C RATIO OF ELEMENTS
0014      RAN = AR/AN2
0015      RCN= CAR/AN2
0016      RHN=HYD/AN2
0017      RON=OX/AN2
0018      RNEN=ANE/AN2
          C
0019      DEL1=0.
0020      DEL2=0.
0021      DEL3=0.
0022      IF (OX.GE.FUEL) GO TO 1
0023      WRITE(LP,97)ITEM
0024      FUEL = OX
0025      1 CONTINUE
          C INITIAL GUESS OF O2,H2O,N2 PARTIAL PRESSURES
0026      XX = .5/((.5*HYD+OX+AN2)*.S+AR)
0027      P(7)=PR*XX*(OX-FUEL)
0028      P(9)=2.*CAR*XX*PR
0029      P(8)=HYD*XX*PR
0030      P(10)= AN2*XX*PR
0031      PAR=2.*P(10)*RAN
0032      PNE=2. * P(10) * RNEN
0033      L= 7
          C ITERATION LOOP TO FIND PARTIAL PRESSURES
0034      IF (P(L).LE..01) P(L)=.01
0035      DO 4 K=1,50

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0036      KOUNT=K
C      CHECK ALL INITIAL PARTIAL PRESSURES FOR NEGATIVE VALUES
0037      DO 41 J=1,10
0038      41 IF (P(J).LT.0.) P(J)=1.E-5
C      OON'T RECALCULATE FREE ENERGY RELATION FOR T KNOWN--IT=1
0039      IF (K.GE.2.AND.IT.EQ.1) GO TO 10
0040      IF (IT.EQ.0.AND.K.EQ.1) T=1670.
0041      CALL THERM(P,T,H,S,CP,F,PR,PAR,PNE,WTM,0)
0042      E(1) = 2.7182818285**(.5*F(8)-.25*F(7)-F(1))
0043      E(2) = 2.7182818285**(.5*F(7)-F(2))
0044      E(3) = 2.7182818285**(.5*F(8)+.25*F(7)-F(3))
0045      E(4) = 2.7182818285**(.5*F(10)+.5*F(7)-F(4))
0046      E(5) = 2.7182818285** (F(9) - .5*F(7) - F(5))
0047      E(6) = 2.7182818285** (F(8) - .5*F(7) - F(6))
C      CALCULATE PARTIAL PRESSURES OF THE ASSUMED KNOWN SPECIES
0048      10 P(1)= SQRT(P(8)/SQRT(P(7))) * E(1)
0049      P(2)= SQRT(P(7)) * E(2)
0050      P(3)=SQRT(P(8)*SQRT(P(7))) * E(3)
0051      P(4)=SQRT(P(10)*P(7)) * E(4)
0052      XX=1./(1.+E(5)/SQRT(P(7)))
0053      P(9)= RCN*(2.*P(10)+P(4))*XX
0054      P(5)= P(9)/SQRT(P(7)) * E(5)
0055      P(6)= P(8)/SQRT(P(7)) * E(6)
0056      PAR = (2. * P(10) + P(4)) * RAN
0057      PNE= (2. * P(10) + P(4)) * RNEN
C
C      DERIVATION OF RELATIONSHIP OF KNOWN SPECIES WITH RESPECT TO GUESS
0058      DO 11 I=1,3
0059      D1(I)=0.
0060      D2(I)=0.
0061      D3(I)=0.
0062      D4(I)=0.
0063      D5(I)=0.
0064      D6(I)=0.
0065      D7(I)=0.
0066      D8(I)=0.
0067      D9(I)=0.
0068      11 D10(I)=0.
0069      D1(1)= -P(1)/P(7)*.25
0070      D1(2)= P(1)/P(8)*.5
0071      D2(1)= P(2)/P(7)*.5
0072      D3(1)= P(3)/P(7)*.25
0073      D3(2)= P(3)/P(8)*.5
0074      D4(1)= P(4)/P(7)*.5
0075      D4(3)=P(4)/P(10)*.5
0076      IF (CAR.EQ.0.0) GO TO 441
0077      D9(1)= RCN*(D4(1)+(2.*P(10)+P(4))*XX*.5*E(5)/P(7)+1.5)*XX
0078      D9(3)= RCN*XX*(2.+D4(3))
0079      D5(1)= P(5)/P(9)*D9(1)-P(5)/P(7)*.5
0080      D5(3)= P(5)/P(9)*D9(3)
0081      441 CONTINUE
0082      D6(1)= -P(6)/P(7)*.5
0083      D6(2)= P(6)/P(8)
0084      D7(1)=1.0
0085      D8(2)=1.0
0086      D10(3)=1.0

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0087      OAR(1)=RAN*D4(1)
0088      OAR(2)=0.
0089      OAR(3)=RAN*(D4(3)+2.)
0090      ONE(1) = RNEN = D4(1)
0091      ONE(2) = 0.0
0092      ONE(3) = RNEN = (D4(3) + 2.)

C
C      DERIVATION OF MATRIX COEFFICIENTS
0093      DO12 I=1,3
0094      A1(I)= D1(I)+O3(I)+2.*D6(I)+2.*D8(I)-RHN*(2.*D10(I)+D4(I))
0095      A2(I)= O2(I)+O3(I)+D4(I)+D5(I)+2.*D7(I)+D8(I)+2.*D9(I)-RON*(2.
      *D10(I)+D4(I))
0096      A3(I)= O1(I)+O2(I)+D3(I)+D4(I)+D5(I)+D6(I)+D7(I)+D8(I)+D9(I)+D10(
      *I)+OAR(I) + ONE(I)
0097      12 CONTINUE
0098      SP1 = P(1)+P(3)+2.*P(6)+2.*P(8)-RHN*(2.*P(10)+P(4))
0099      SP2 = P(2)+P(3)+P(4)+P(5)+2.*P(7)+P(8)+2.*P(9)-RON*(2.*P(10)+P(4
      *I))
0100      SP3 =0.
0101      DO 13 I=1,10
0102      13 SP3 =SP3 +P(I)
0103      SP3=SP3-PR*PAR + PNE

C
C      SOLUTION OF MATRIX
0104      DEN= A1(1)*(A2(2)*A3(3)-A3(2)*A2(3))-A2(1)*(A1(2)*A3(3)-A3(2)*
      *A1(3))+A3(1)*(A1(2)*A2(3)-A2(2)*A1(3))
0105      DEN=1./DEN
0106      XN1 =SP1*(A3(2)*A2(3)-A2(2)*A3(3))+SP2*(A1(2)*A3(3)-A1(3)*A3(2))+
      *SP3*(A1(3)*A2(2)-A1(2)*A2(3))
0107      XN2 =SP1*(A2(1)*A3(3)-A3(1)*A2(3))+SP2*(A3(1)*A1(3)-A1(1)*A3(3))+
      *SP3*(A1(1)*A2(3)-A2(1)*A1(3))
0108      XN3 =SP1*(A3(1)*A2(2)-A2(1)*A3(2))+SP2*(A1(1)*A3(2)-A3(1)*A1(2))+
      *SP3*(A2(1)*A1(2)-A1(1)*A2(2))

C
C      CALCULATION OF PARTIAL PRESS CORRECTION AND NEW GUESSED PART PRESS
0109      DEL1= XN1 *DEN
0110      DEL2= XN2 *DEN
0111      DEL3=XN3*DEN
0112      P(L)=P(L)+DEL1
0113      P(8)=P(8)+DEL2
0114      P(10)=P(10)+DEL3

C
C      FIND ENTHALPY FOR ITERATION TO FIND TEMP.
0115      7 CONTINUE
0116      IF(17)18,18,6
0117      18 CALL THERM(P,T,H ,5,CP,F,PR,PAR,PNE,WTN,1)
0118      80 CONTINUE
0119      IF (ICT.GT.0) GO TO 85
0120      DELT = ((H0-H)/CP)/1.8
0121      IF (DFLT*DELT) 81,81,82
0122      82 T=T+DELT
0123      GO TO 85
0124      81 T=T+DELT
0125      ICT=2
0126      85 ICT=ICT-1
0127      DELTL=DELT

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0128      IF (T.LE.300.) T=300.0
0129      IF (T.GE.5000.) T=5000.
      C
      C      ITERATION CONTRDL--TEMP.WITHIN 1 DEG OR PRESS WITHIN DELL
0130      IF (ABS(H0-H) -.1* CP) 6.6,4
0131      6 IF (ABS(DELL) -(0.01*DELL)) 22,22,4
0132      22 IF (ABS(DELL2) - DELL) 23,23,4
0133      23 IF (ABS(DELL3) - DELL) 5,5,4
0134      4 CONTINUE
0135      5 CONTINUE
0136      PHOLD=PR
      C
      C      WRITE(LP,3) (P(I), I=1,10)
0137      3 FORMAT(10F7,4)
      C      CALL THERM(P,T,H,S,CP,F,PR,PAR,PNE,WTM,1)
      C      WRITE(LP,3) (P(I), I=1,10)
      C      3 FORMAT(10F7,4)
0138      TT=T*1.8
0139      NT=KOUNT
0140      RETURN
0141      97 FORMAT(1H ,I4,2X,6HPROP .2X,36H THIS CASE HAS TOO LITTLE O2 TO RU
      *N )
0142      END

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FORTRAN IV G LEVEL 21

THERM

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0001      SUBROUTINE THERM(BLP,T,H,S,CP,F,PR,PAR,PNE,WTM,KT)
0002      COMMON/CATHY/XN2,XO2,XAR,XCO2,XNE,MWA1R,Y(14)
0003      DIMENSION ALP(12),CX(72),CY(72),CTT(144),HX(12),SX(12),CPX(12),
          IC1(4),C2(4),CT(72),F(10),CF(4),C3(4)
0004      DIMENSION BLP(10)
0005      EQUIVALENCE(CTT(1),CT(1)),(CTT(73),CX(1))
0006      DO 50 I=1,6
0007      50 ALP(I) = BLP(I)
0008      ALP(7) = BLP(10)
0009      ALP(8) = BLP(7)
0010      ALP(9) = PAR
0011      ALP(10) = BLP(9)
0012      ALP(11) = PNE
0013      ALP(12) = BLP(8)
0014      DO 51 I=1,12
0015      51 ALP(I) = ALP(I) / PR
0016      CP=0.0
0017      H = 0.0
0018      S = 0.0
0019      IF(KT)400,100,200
          C  CALCULATE FREE ENERGY
0020      100 CALL COEFF(1,CT)
0021      T = T * 1.8
0022      DO 201 K=1,10
0023      F(K) = 0.0
0024      KF=4*(K-1)
0025      DO 300 J=1,4
0026      KFF = KF + J
0027      TX = T ** (J-1)
0028      300 CF(J)=CT(KFF)*TX
0029      DO 301 J=1,4
0030      301 F(K) = F(K) + CF(J)
0031      201 CONTINUE
0032      F10 = F(10)
0033      F(10) = F(7)
0034      F(7) = F(8)
0035      F(8) = F10
0036      DO 81 I=1,10
0037      81 F(I) = (F(I)/T)*(1.8/1.987165)
0038      T=T/1.8
0039      RETURN
          C  CALCULATE MICHEMICAL + SENSIBLE ENTHALPY,S,CP
0040      200 CALL COEFF(2,CT)
0041      CALL COEFF(3,CX)
0042      CALL COEFF(4,CY)
0043      T = T*1.8
0044      DO 2 K=1,12
0045      HX(K) = 0
0046      SX(K) = 0
0047      CPX(K) = 0
0048      KA = 0
0049      IF(K=7)20,21,21
0050      21 IF(T-2700.0)20,20,27
0051      27 KA = 24
0052      20 KK = 4*(K-1) + KA
0053      DO 3 J=1,4

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0054      KKK = KK+J
0055      TX = T ** (J-1)
0056      C1(J) = CT(KKK) * TX
0057      C2(J) = CX(KKK) * TX
0058      3 C3(J) = CY(KKK) * TX
0059      DO 30 J=1,4
0060      HX(K) = HX(K) + C1(J)
0061      SX(K) = SX(K) + C2(J)
0062      30 CPX(K) = CPX(K) + C3(J)
0063      IF(ALP(K).LE.0.)GO TO 11
0064      SX(K) = SX(K) - 1.987165 * ALOG(ALP(K) * PR)
0065      GO TO 12
0066      11 SX(K)=0.
0067      12 CONTINUE
0068      IF(K-6)25,23,25
0069      23 CPX(K) = CPX(K) + 0.439912E-13 * T **4.0
0070      25 IF(K-7)35,29,35
0071      29 IF(T-2700.0)31,31,35
0072      31 SX(K) = SX(K) + 0.6848142E-12 * T ** 4.0
0073      35 CONTINUE
0074      H = H + ALP(K) * HX(K)
0075      S = S + ALP(K) * SX(K)
0076      CP = CP + ALP(K) * CPX(K)
0077      2 CONTINUE
0078      WTM = ALP(1) * Y(7) + ALP(2) * Y(8) + ALP(3) * Y(9) + ALP(4) *
1      Y(10) + ALP(5) * Y(11) + ALP(6) * Y(12) + ALP(7) * Y(1) +
1      ALP(8) * Y(2) + ALP(9) * Y(3) + ALP(10)*Y(4) + ALP(11) * Y(5)
1 + ALP(12) * Y(6)
0079      H = H / WTM
0080      S = S / WTM
0081      CP = CP / WTM
0082      T = T / 1.8
0083      400 CONTINUE
0084      RETURN
0085      END

```

FORTRAN IV G LEVEL 21

FUELM

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```

0001      SUBROUTINE FUELM(A,B,PHI,XX,XM,HV,H)
0002      C      CALCULATES ENTHALPY OF FUEL FROM HEATING VALUE.
0003      C      COMMON/CATHY/XN2,XO2,XAR,XCO2,XNE,MWAIR,Y(14),DUMMY(12)
0004      C      FUEL AND AIR ARE AT 536 DEGREES R
0005      C      TFUEL = 536.7
0006      C      EQ. FOR CPFUEL FROM NASA-TN-3276
0007      CPFUEL = 0.0005*(TFUEL-459.67)*0.44
0008      HAIR = -1.8680522
0009      PCTF = (Y(13) * A + Y(7) * B)/(Y(13) * A + Y(7) * B + Y(8) * 2.0 +
1      XO2 * Y(14) * 2.0 + XN2 * Y(13) * XAR + Y(5) * XNE)
0007      WTMF = Y(13) * A + Y(7) * B
0008      HF = HV + (94054.0 * (A-XCO2) + 57797.9 * (B/2.0))*(1.8/WTMF)
0009      * + CPFUEL * (TFUEL-536.7)
0010      H = PCTF * HF + (1.0 - PCTF) * HAIR
0011      RETURN
0011      END

```

FORTRAN IV G LEVEL 21

HMIKP

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```

0001      FUNCTION HMIKP(PA,TR,MID,LP,ITEM)
0002      REAL MWAIR
0003      COMMON/CATHY/AMF(5),MWAIR,Y(14)
          C          CALCULATE ENTHALPY WITH PRESSURE
          C          CORRECTION
0004      CH = 82.056
          C      GAS CONSTANT(ATM-CM**3)/(GM-MOLE-(DEG)K)
0005      T = TR/1.8
0006      IF(T-166.)3,4,4
0007      3 T=166.0
0008      4 OHM = 0.0
0009      DELT = (CH * T / PA) / 10000.0
0010      CTR = 0.0
0011      DO 20 I=1,5
0012      BI = BBB(I,I,TR)
0013      CI = CCC(I,I,TR)
0014      BPI = BBB(2,I,TR)
0015      CPI = CCC(2,I,TR)
          C      CALCULATION OF SPECIFIC VOLUME(I)
0016      VIG = CH * T / PA * BI * CI
0017      14 VI = CH * T / PA * (1.0 * BI / VIG * CI/(VIG * VIG))
0018      IF(ABS(VI-VIG)-DELT)10,10,15
0019      15 CTR = CTR + 1.0
0020      VIG = VI
0021      IF(CTR-25.0)14,16,16
0022      16 VI = CH * T / PA
0023      10 CONTINUE
0024      OH = 1.987165 / Y(I) *
          I      TR * ( 1.0 / VI * (BI - BPI) * 1.0/VI * 1.0/VI * (CI - 0.5 *
          2CPI))
0025      20 OHM = OH * AMF(I) * OHM
0026      HMIKP = MID * OHM
0027      RETURN
0028      END

```

FORTRAN IV G LEVEL 21

SMIXP

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```

0001      FUNCTION SMIXP(PA,TR,SID,LP,ITEM)
0002      REAL MWAIR
0003      COMMON/CATHY/AMF(5),MWAIR,Y(I4)
          C
          C          CALCULATE ENTROPY WITH PRESSURE
          C          CORRECTION
0004      CS = 82.056
          C
          C      GAS CONSTANT (ATM-CM**3)/(GM-MOLE-(OEG)K)
          C      T = TR/1.8
0005      T = TR/1.8
0006      IF (T-166.)3,4,4
0007      3 T=166.0
0008      4 DSM = 0.0
0009      DELT = (CS * T/PA) / 10000.0
0010      00 20 I = 1.5
0011      B1 = BBB(1,I,TR)
0012      C1 = CCC(1,I,TR)
0013      BPI = BBB(2,I,TR)
0014      CPI = CCC(2,I,TR)
0015      CTR = 0.0
          C
          C      CALCULATION OF SPECIFIC VOLUME(I)
0016      VIG = CS * T / PA + B1 + C1
0017      14 VI = CS * T / PA * (1.0 + B1 / VIG + C1 / (VIG * VIG))
0018      IF (ABS(VI-VIG)-DELT)16,16,15
0019      15 CTR = CTR + 1.0
0020      VIG = VI
0021      IF (CTR-25.0)14,16,16
0022      16 VI = CS * T / PA
0023      18 CONTINUE
0024      OS = -1.987165 / Y(I) *
          1
          2 (B1 + B1) / 2.0 + C1/2.0 + BPI/VI + (1.0/VI) * (1.0/VI) * (
0025      20 OSM = OSM + OS * AMF(I)
0026      SMIXP = SID + OSM
0027      RETURN
0028      END

```


FORTRAN IV G LEVEL 21

CPMIXP

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```

0001      FUNCTION CPMIXP(PA,TR,CPID,LP,ITEM)
0002      C      CALCULATION OF SPECIFIC HEAT WITH PRESSURE CORRECTION.
0003      COMMON/CATHY/AMF(5),MWAIR,Y(14)
0004      REAL MWAIR
0005      CI = 82.056
0006      C      GAS CONSTANT CI(ATM-CM**3)/GM-MOLE = (D5G)K
0007      T = TR/1.8
0008      IF(T-166.)3,4,4
0009      3 T=166.0
0010      4 OCP = 0.0
0011      DELT = (CI * T / PA ) /10000.0
0012      DO 20 I=1,5
0013      BP1 = BBB(2,I,TR)
0014      CPI = CCC(2,I,TR)
0015      BI = BBB(1,I,TR)
0016      CI = CCC(1,I,TR)
0017      CPPI = CCC(3,I,TR)
0018      BPPI = BBB(3,I,TR)
0019      CTR = 0.0
0020      C      CALCULATION OF SPECIFIC VOLUME(I)
0021      VIG = CI * T / PA + BI * CI
0022      14 VI = CI * T / PA * (1.0 + BI / VIG + CI/(VIG * VIG))
0023      IF(ABS(VI-VIG)-DELT)18,18,15
0024      15 CTR = CTR + 1.0
0025      VIG = VI
0026      IF(CTR-25.0)14,16,16
0027      16 VI = CI * T / PA
0028      18 CONTINUE
0029      OCPI = (-1.987165) / Y(I)
0030      1      * ( BPPI/ VI - 1.0/VI + 1.0/VI * ((BI - BP1) *
0031      2 (BI - BP1) - CI * CPI - 0.5 * CPPI))
0032      20 OCP = OCP + OCPI * AMF(I)
0033      CPMIXP = CPID + OCP
0034      RETURN
0035      ENO

```

FORTRAN IV G LEVEL 21

HSCP

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```

0001      SUBROUTINE HSCP(TX,K,KK,M)
          C      CURVE FIT ROUTINE FOR CONSTITUENT PROPERTIES-300R-900R
          C      - AEDC -TR -75-          -REF.20
0002      DIMENSION C1(5,52,4), C2(5,14,4), C3(3,11,4)
0003      DIMENSION X1(95),X2(95),X3(95),X4(95),X5(95),X6(95),X7(95),X8(95),
          X9(95),X10(95),X11(90),X12(95),X13(95),X14(90),X15(95),X16(37)
0004      EQUIVALENCE (X1(1),C1(1)),(X2(1),C1(96)),(X3(1),C1(191)),
          1(X4(1),C1(286)),(X5(1),C1(381)),(X6(1),C1(476)),(X7(1),C1(571)),
          2(X8(1),C1(666)),(X9(1),C1(761)),(X10(1),C1(856)),
          3(X11(1),C1(951)),(X12(1),C2(1)),(X13(1),C2(96)),(X14(1),C2(191)),
          4(X15(1),C3(1)),(X16(1),C3(96))
0005      REAL INC
0006      DATA X 1/
          * 0.69300E 00, 0.69400E 00, 0.0          , 0.12518E 04, 0.78600E 00,
          * 0.76300E 00, 0.76300E 00, 0.90000E 01, 0.13777E 04, 0.86600E 00,
          * 0.83300E 00, 0.83300E 00, 0.50600E 03, 0.15040E 04, 0.94600E 00,
          * 0.90200E 00, 0.90300E 00, 0.10030E 04, 0.16312E 04, 0.10250E 01,
          * 0.97200E 00, 0.97200E 00, 0.15000E 04, 0.17594E 04, 0.11050E 01,
          * 0.10410E 01, 0.10420E 01, 0.19960E 04, 0.18888E 04, 0.11840E 01,
          * 0.11110E 01, 0.11110E 01, 0.24930E 04, 0.20197E 04, 0.12640E 01,
          * 0.11800E 01, 0.11810E 01, 0.29900E 04, 0.21522E 04, 0.13440E 01,
          * 0.12500E 01, 0.12500E 01, 0.34870E 04, 0.22864E 04, 0.14230E 01,
          * 0.13190E 01, 0.13200E 01, 0.39840E 04, 0.24227E 04, 0.15030E 01,
          * 0.13890E 01, 0.13900E 01, 0.44800E 04, 0.25608E 04, 0.15830E 01,
          * 0.14590E 01, 0.14590E 01, 0.49770E 04, 0.27010E 04, 0.16620E 01,
          * 0.15280E 01, 0.15290E 01, 0.54740E 04, 0.28434E 04, 0.17420E 01,
          * 0.15980E 01, 0.15990E 01, 0.0          , 0.29879E 04, 0.18220E 01,
          * 0.16670E 01, 0.16680E 01, 0.0          , 0.31345E 04, 0.19020E 01,
          * 0.17370E 01, 0.17380E 01, 0.0          , 0.32834E 04, 0.19820E 01,
          * 0.18060E 01, 0.18080E 01, 0.0          , 0.34343E 04, 0.20610E 01,
          * 0.18760E 01, 0.18780E 01, 0.0          , 0.35873E 04, 0.21410E 01,
          * 0.19460E 01, 0.19480E 01, 0.0          , 0.37424E 04, 0.22220E 01 /
0007      DATA X 2/
          * 0.20150E 01, 0.20180E 01, 0.0          , 0.38995E 04, 0.23020E 01,
          * 0.20720E 01, 0.20750E 01, 0.0          , 0.40586E 04, 0.23670E 01,
          * 0.20850E 01, 0.20880E 01, 0.0          , 0.42198E 04, 0.23820E 01,
          * 0.21540E 01, 0.21580E 01, 0.0          , 0.43828E 04, 0.24620E 01,
          * 0.22240E 01, 0.22290E 01, 0.0          , 0.45476E 04, 0.25430E 01,
          * 0.22940E 01, 0.22990E 01, 0.0          , 0.47144E 04, 0.26230E 01,
          * 0.23630E 01, 0.23700E 01, 0.0          , 0.48829E 04, 0.27040E 01,
          * 0.24330E 01, 0.24410E 01, 0.0          , 0.50532E 04, 0.27850E 01,
          * 0.25030E 01, 0.25120E 01, 0.0          , 0.52254E 04, 0.28660E 01,
          * 0.25730E 01, 0.25830E 01, 0.0          , 0.53991E 04, 0.29470E 01,
          * 0.26420E 01, 0.26550E 01, 0.0          , 0.55745E 04, 0.30280E 01,
          * 0.27120E 01, 0.27260E 01, 0.0          , 0.57515E 04, 0.31100E 01,
          * 0.27820E 01, 0.27980E 01, 0.0          , 0.59300E 04, 0.31920E 01,
          * 0.28520E 01, 0.28700E 01, 0.0          , 0.61101E 04, 0.32740E 01,
          * 0.29220E 01, 0.29430E 01, 0.0          , 0.62918E 04, 0.33560E 01,
          * 0.29920E 01, 0.30150E 01, 0.0          , 0.64749E 04, 0.34380E 01,
          * 0.30620E 01, 0.30880E 01, 0.0          , 0.66607E 04, 0.35210E 01,
          * 0.31320E 01, 0.31610E 01, 0.0          , 0.68454E 04, 0.36040E 01,
          * 0.32030E 01, 0.32340E 01, 0.0          , 0.70327E 04, 0.36870E 01 /
0008      DATA X 3/
          * 0.32730E 01, 0.33070E 01, 0.0          , 0.72215E 04, 0.37700E 01,
          * 0.33440E 01, 0.33810E 01, 0.0          , 0.74116E 04, 0.38540E 01,
          * 0.34140E 01, 0.34550E 01, 0.0          , 0.76029E 04, 0.39370E 01

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* 0.34850E 01, 0.35290E 01, 0.0      , 0.77954E 04, 0.40210E 01,
* 0.35560E 01, 0.36040E 01, 0.0      , 0.79894E 04, 0.41060E 01,
* 0.36260E 01, 0.36780E 01, 0.0      , 0.81844E 04, 0.41900E 01,
* 0.36970E 01, 0.37530E 01, 0.0      , 0.83807E 04, 0.42750E 01,
* 0.37680E 01, 0.38280E 01, 0.0      , 0.85782E 04, 0.43600E 01,
* 0.38400E 01, 0.39040E 01, 0.0      , 0.87768E 04, 0.44450E 01,
* 0.39110E 01, 0.39800E 01, 0.0      , 0.89766E 04, 0.45310E 01,
* 0.39830E 01, 0.40550E 01, 0.0      , 0.91774E 04, 0.46170E 01,
* 0.40540E 01, 0.41320E 01, 0.0      , 0.93796E 04, 0.47030E 01,
* 0.41260E 01, 0.42080E 01, 0.0      , 0.0      , 0.47890E 01,
* 0.0      , 0.0      , 0.0      , 0.0      , 0.0      ,
* 0.70000E-02, 0.68500E-02, 0.48119E 01, 0.12566E 02, 0.80000E-02,
* 0.70000E-02, 0.70000E-02, 0.49700E 01, 0.12606E 02, 0.80000E-02,
* 0.70000E-02, 0.70000E-02, 0.49700E 01, 0.12663E 02, 0.80000E-02,
* 0.69500E-02, 0.70000E-02, 0.49700E 01, 0.12760E 02, 0.79500E-02,
* 0.69500E-02, 0.69500E-02, 0.49700E 01, 0.12865E 02, 0.79500E-02 /
DATA X 4/
* 0.69500E-02, 0.69500E-02, 0.49700E 01, 0.13003E 02, 0.80000E-02,
* 0.69500E-02, 0.69500E-02, 0.49700E 01, 0.13163E 02, 0.80000E-02,
* 0.69500E-02, 0.69500E-02, 0.49700E 01, 0.13328E 02, 0.79999E-02,
* 0.69500E-02, 0.70000E-02, 0.49700E 01, 0.13519E 02, 0.80000E-02,
* 0.70000E-02, 0.70000E-02, 0.49700E 01, 0.13716E 02, 0.80000E-02,
* 0.70000E-02, 0.70000E-02, 0.49700E 01, 0.13913E 02, 0.80000E-02,
* 0.69999E-02, 0.69999E-02, 0.49700E 01, 0.14130E 02, 0.80000E-02,
* 0.69500E-02, 0.70000E-02, 0.49700E 01, 0.14343E 02, 0.80000E-02,
* 0.69500E-02, 0.70000E-02, 0.0      , 0.14552E 02, 0.80000E-02,
* 0.69500E-02, 0.70000E-02, 0.0      , 0.14779E 02, 0.80000E-02,
* 0.69500E-02, 0.70000E-02, 0.0      , 0.14987E 02, 0.80000E-02,
* 0.70000E-02, 0.70000E-02, 0.0      , 0.15194E 02, 0.79500E-02,
* 0.70000E-02, 0.70000E-02, 0.0      , 0.15411E 02, 0.80500E-02,
* 0.70000E-02, 0.70001E-02, 0.0      , 0.15610E 02, 0.80196E-02,
* 0.69709E-02, 0.69999E-02, 0.0      , 0.15813E 02, 0.79895E-02,
* 0.70078E-02, 0.70000E-02, 0.0      , 0.16017E 02, 0.80000E-02,
* 0.69955E-02, 0.70199E-02, 0.0      , 0.16212E 02, 0.80464E-02,
* 0.70000E-02, 0.70209E-02, 0.0      , 0.16392E 02, 0.80519E-02,
* 0.70000E-02, 0.70500E-02, 0.0      , 0.16577E 02, 0.80500E-02 /
DATA X 5/
* 0.69999E-02, 0.71000E-02, 0.0      , 0.16772E 02, 0.81000E-02,
* 0.70000E-02, 0.71000E-02, 0.0      , 0.16943E 02, 0.81000E-02,
* 0.70000E-02, 0.71000E-02, 0.0      , 0.17124E 02, 0.81000E-02,
* 0.70000E-02, 0.70999E-02, 0.0      , 0.17295E 02, 0.81000E-02,
* 0.70000E-02, 0.71001E-02, 0.0      , 0.17458E 02, 0.81000E-02,
* 0.70000E-02, 0.71500E-02, 0.0      , 0.17625E 02, 0.81500E-02,
* 0.70000E-02, 0.71999E-02, 0.0      , 0.17777E 02, 0.82000E-02,
* 0.70000E-02, 0.72000E-02, 0.0      , 0.17932E 02, 0.82000E-02,
* 0.70000E-02, 0.72001E-02, 0.0      , 0.18087E 02, 0.82000E-02,
* 0.70000E-02, 0.72500E-02, 0.0      , 0.18219E 02, 0.82001E-02,
* 0.70000E-02, 0.73000E-02, 0.0      , 0.18469E 02, 0.82500E-02,
* 0.70000E-02, 0.73000E-02, 0.0      , 0.18525E 02, 0.82999E-02,
* 0.70001E-02, 0.73000E-02, 0.0      , 0.18581E 02, 0.83000E-02,
* 0.70500E-02, 0.73000E-02, 0.0      , 0.18830E 02, 0.83000E-02,
* 0.70500E-02, 0.73500E-02, 0.0      , 0.18947E 02, 0.83000E-02,
* 0.70500E-02, 0.74000E-02, 0.0      , 0.19070E 02, 0.83500E-02,
* 0.71000E-02, 0.74000E-02, 0.0      , 0.19191E 02, 0.83500E-02,
* 0.71000E-02, 0.74000E-02, 0.0      , 0.19333E 02, 0.84500E-02,
* 0.71000E-02, 0.74500E-02, 0.0      , 0.19447E 02, 0.84500E-02 /

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* 0.71000E-02, 0.75000E-02, 0.0      , 0.19561E 02, 0.85000E-02,
* 0.71000E-02, 0.75000E-02, 0.0      , 0.19697E 02, 0.85000E-02,
* 0.71000E-02, 0.75500E-02, 0.0      , 0.19808E 02, 0.85000E-02,
* 0.71500E-02, 0.76000E-02, 0.0      , 0.19921E 02, 0.85000E-02,
* 0.71500E-02, 0.76000E-02, 0.0      , 0.20025E 02, 0.86000E-02,
* 0.71500E-02, 0.76000E-02, 0.0      , 0.20156E 02, 0.86000E-02,
* 0.71999E-02, 0.76000E-02, 0.0      , 0.20264E 02, 0.85999E-02,
* 0.72000E-02, 0.76000E-02, 0.0      , 0.0      , 0.86001E-02,
* 0.0      , 0.0      , 0.0      , 0.0      , 0.0      ,
* 0.37253E-09, 0.14901E-08, 0.30928E-05, 0.30143E-02, 0.37253E-09,
* 0.11176E-08, 0.18626E-08, 0.28610E-07, 0.33064E-02, 0.74506E-09,
* 0.24998E-04, 0.22352E-08, 0.28610E-07, 0.73268E-02, 0.25006E-04,
* 0.15006E-04, 0.24998E-04, 0.28610E-07, 0.68241E-02, 0.15004E-04,
* -0.15009E-04, 0.15002E-04, 0.29998E-03, 0.80565E-02, 0.20012E-04,
* 0.14995E-04, 0.15019E-04, 0.28610E-07, 0.99821E-02, 0.25332E-07,
* -0.14991E-04, 0.15021E-04, 0.19073E-07, 0.91564E-02, 0.11176E-08,
* 0.15019E-04, 0.19988E-04, 0.95367E-08, 0.10224E-01, 0.29991E-04,
* -0.20021E-04, 0.11176E-08, 0.28610E-07, 0.10937E-01, 0.11176E-08,
* 0.24587E-07, 0.11176E-08, 0.29998E-03, 0.10333E-01, 0.11176E-08 /

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0012

DATA X 7/

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* 0.14901E-08, 0.29973E-04, 0.28610E-07, 0.10767E-01, 0.29983E-04,
* -0.24967E-04, 0.15274E-07, 0.19073E-07, 0.11654E-01, 0.11176E-08,
* 0.14992E-04, 0.20117E-07, 0.0      , 0.10010E-01, 0.74506E-09,
* -0.14991E-04, 0.30012E-04, 0.0      , 0.11176E-01, 0.37253E-09,
* 0.14992E-04, 0.28685E-07, 0.0      , 0.10946E-01, 0.11176E-08,
* -0.19988E-04, 0.0      , 0.0      , 0.93161E-02, 0.24985E-04,
* 0.11176E-08, 0.0      , 0.0      , 0.11195E-01, 0.49986E-05,
* 0.11176E-08, 0.18999E-07, 0.0      , 0.97370E-02, 0.18031E-04,
* -0.27081E-04, 0.15646E-07, 0.0      , 0.96234E-02, 0.28677E-05,
* 0.39530E-05, 0.22055E-05, 0.0      , 0.10141E-01, 0.63939E-05,
* 0.36842E-04, 0.32052E-04, 0.0      , 0.90042E-02, 0.14984E-03,
* -0.29083E-04, 0.60603E-05, 0.0      , 0.92697E-02, 0.14472E-04,
* 0.20117E-07, 0.20793E-04, 0.0      , 0.84900E-02, 0.14610E-04,
* 0.14901E-08, 0.19982E-04, 0.0      , 0.97870E-02, 0.20002E-04,
* -0.29964E-04, 0.11176E-08, 0.0      , 0.86868E-02, 0.11176E-08,
* 0.11176E-08, 0.11176E-08, 0.0      , 0.75607E-02, 0.74506E-09,
* 0.74506E-09, 0.18254E-07, 0.0      , 0.95245E-02, 0.29057E-07,
* 0.28312E-07, 0.10803E-07, 0.0      , 0.66376E-02, 0.37253E-09,
* -0.30012E-04, 0.24994E-04, 0.0      , 0.88608E-02, 0.49964E-05 /

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0013

DATA X 8/

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* 0.28685E-07, 0.19983E-04, 0.0      , 0.70419E-02, 0.99946E-05,
* 0.0      , 0.15274E-07, 0.0      , 0.76401E-02, 0.11176E-08,
* 0.0      , 0.14901E-08, 0.0      , 0.76996E-02, 0.11176E-08,
* 0.27940E-07, 0.24971E-04, 0.0      , 0.96481E-02, 0.20489E-07,
* 0.0      , 0.20011E-04, 0.0      , 0.37888E-02, 0.50206E-05,
* 0.37253E-09, 0.11176E-08, 0.0      , 0.27516E-01, 0.10015E-04,
* 0.10431E-07, 0.74506E-09, 0.0      , -0.21849E-01, 0.85682E-08,
* 0.24943E-04, 0.37253E-09, 0.0      , 0.20108E-01, 0.11176E-08,
* -0.14980E-04, 0.50012E-05, 0.0      , 0.27939E-02, 0.11176E-08,
* 0.15005E-04, 0.10005E-04, 0.0      , 0.54031E-02, 0.24985E-04,
* -0.20011E-04, 0.11176E-08, 0.0      , 0.45598E-02, 0.15800E-04,
* 0.11176E-08, 0.27940E-07, 0.0      , 0.53101E-02, 0.50079E-05,
* 0.11176E-08, 0.24989E-04, 0.0      , 0.74905E-02, 0.14996E-04,
* -0.30011E-04, 0.19973E-04, 0.0      , 0.35721E-02, 0.20011E-04,
* 0.11176E-08, 0.14901E-08, 0.0      , 0.83603E-02, 0.11176E-08,

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*0.14991E-05,-0.50027E-06, 0.0      , 0.54932E-05,-0.74506E-10.
* 0.99979E-06,-0.74506E-10, 0.0      , -0.36316E-04,-0.99860E-06.
*0.10010E-05, 0.20003E-05, 0.0      , 0.13763E-03,-0.52154E-09.
* 0.14984E-05,-0.20014E-05, 0.0      , -0.52948E-04, 0.40978E-09.
*0.74506E-10, 0.13411E-08, 0.0      , 0.86670E-04,-0.74506E-10.
* 0.40978E-09, 0.40973E-09, 0.0      , 0.0      , -0.49889E-06.
* 0.0      , 0.0      , 0.0      , 0.0      , 0.0      /

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DATA X12/

```

* 0.38170E 02, 0.41345E 02, 0.71400E 01, 0.42758E 02, 0.36396E 02.
* 0.42992E 02, 0.46218E 02, 0.71800E 01, 0.47769E 02, 0.41916E 02.
* 0.45770E 02, 0.49014E 02, 0.90500E 01, 0.51072E 02, 0.45106E 02.
* 0.45813E 02, 0.49047E 02, 0.10640E 02, 0.51127E 02, 0.45155E 02.
* 0.47818E 02, 0.51091E 02, 0.12080E 02, 0.53830E 02, 0.47484E 02.
* 0.49386E 02, 0.52722E 02, 0.13280E 02, 0.56122E 02, 0.49334E 02.
* 0.50685E 02, 0.54698E 02, 0.14280E 02, 0.58126E 02, 0.50891E 02.
* 0.51806E 02, 0.55297E 02, 0.15170E 02, 0.59910E 02, 0.52249E 02.
* 0.52798E 02, 0.56361E 02, 0.15980E 02, 0.61522E 02, 0.53464E 02.
* 0.53692E 02, 0.57320E 02, 0.16720E 02, 0.62992E 02, 0.54570E 02.
* 0.0      , 0.0      , 0.17410E 02, 0.0      , 0.0      ,
* 0.0      , 0.0      , 0.18070E 02, 0.0      , 0.0      ,
* 0.0      , 0.0      , 0.18700E 02, 0.0      , 0.0      ,
* 0.0      , 0.0      , 0.0      , 0.0      , 0.0      ,
* 0.58178E-01, 0.58152E-01, 0.23081E-01, 0.58339E-01, 0.66549E-01.
* 0.32340E-01, 0.32470E-01, 0.20129E-01, 0.36818E-01, 0.37253E-01.
* 0.23941E-01, 0.23878E-01, 0.16850E-01, 0.30285E-01, 0.27234E-01.
* 0.21529E-01, 0.21688E-01, 0.15092E-01, 0.28413E-01, 0.24710E-01.
* 0.17679E-01, 0.18278E-01, 0.13371E-01, 0.25040E-01, 0.20789E-01 /

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DATA X13/

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* 0.13769E-01, 0.14525E-01, 0.10629E-01, 0.21044E-01, 0.16430E-01.
* 0.11787E-01, 0.12603E-01, 0.92143E-02, 0.18663E-01, 0.14233E-01.
* 0.10378E-01, 0.11143E-01, 0.84111E-02, 0.16795E-01, 0.12656E-01.
* 0.93121E-02, 0.10001E-01, 0.76691E-02, 0.15278E-01, 0.11463E-01.
* 0.85026E-02, 0.91142E-02, 0.70499E-02, 0.14056E-01, 0.10586E-01.
* 0.0      , 0.0      , 0.67125E-02, 0.0      , 0.0      ,
* 0.0      , 0.0      , 0.64501E-02, 0.0      , 0.0      ,
* 0.0      , 0.0      , 0.61500E-02, 0.0      , 0.0      ,
* 0.0      , 0.0      , 0.0      , 0.0      , 0.0      ,
*0.40361E-04,-0.40848E-04,-0.77265E-03,-0.31659E-04,-0.47519E-04.
*0.37794E-04,-0.37315E-04,-0.10091E-04,-0.30206E-04,-0.43164E-04.
* 0.17000E-03, 0.15203E-03,-0.10925E-04, 0.11540E-03, 0.15985E-03.
*0.58597E-05,-0.33331E-05,-0.35603E-05,-0.77686E-05,-0.33868E-05.
*0.20860E-04,-0.21507E-04,-0.13714E-04,-0.23646E-04,-0.25080E-04.
*0.35399E-05,-0.37267E-05,-0.47140E-05,-0.63094E-05,-0.38276E-05.
*0.32197E-05,-0.37805E-05,-0.13971E-05,-0.59986E-05,-0.38131E-05.
*0.30831E-05,-0.36685E-05,-0.19137E-05,-0.50714E-05,-0.32553E-05.
*0.30690E-05,-0.34713E-05,-0.18855E-05,-0.51110E-05,-0.33221E-05.
*0.31018E-05,-0.35350E-05,-0.11237E-05,-0.48102E-05,-0.31118E-05 /

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0019

DATA X14/

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* 0.0      , 0.0      , -0.75072E-06, 0.0      , 0.0      ,
* 0.0      , 0.0      , -0.15002E-05, 0.0      , 0.0      ,
* 0.0      , 0.0      , -0.15013E-05, 0.0      , 0.0      ,
* 0.0      , 0.0      , 0.0      , 0.0      , 0.0      ,
*0.59220E-06,-0.58375E-06,-0.89876E-05,-0.50628E-06,-0.65973E-06.
*0.33915E-07,-0.43852E-07,-0.42040E-07,-0.20882E-07,-0.53501E-07.
*0.29616E-03,-0.26809E-03, 0.14243E-07,-0.22392E-03,-0.30344E-03.
*0.89275E-07,-0.91442E-07,-0.33627E-07,-0.60635E-07,-0.10811E-06.

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      * 0.47354E-08, 0.18288E-07, 0.0, , 0.24433E-07, 0.21892E-07,
      * -0.42454E-07, -0.39231E-07, -0.15716E-07, -0.37324E-07, -0.47725E-07,
      * -0.25506E-07, -0.23469E-07, -0.17457E-07, -0.22272E-07, -0.27134E-07,
      * -0.14973E-07, -0.13582E-07, -0.11977E-07, -0.16753E-07, -0.18055E-07,
      * -0.65234E-08, -0.64328E-08, -0.80682E-08, -0.66679E-08, -0.71093E-08,
      * -0.42401E-08, -0.40766E-08, -0.37551E-08, -0.54486E-08, -0.54412E-08,
      * 0.0, , 0.0, , -0.37443E-08, 0.0, , 0.0, ,
      * 0.0, , 0.0, , -0.74506E-12, 0.0, , 0.0, ,
      * 0.0, , 0.0, , 0.29802E-11, 0.0, , 0.0, ,
      * 0.0, , 0.0, , 0.0, , 0.0, , 0.0, /
0020 DATA x15/
      * 0.69580E 01, 0.69810E 01, 0.79610E 01, 0.69610E 01, 0.77340E 01,
      * 0.79690E 01, 0.70200E 01, 0.88740E 01, 0.80250E 01, 0.70230E 01,
      * 0.88960E 01, 0.80270E 01, 0.71960E 01, 0.98770E 01, 0.81860E 01,
      * 0.74310E 01, 0.10666E 02, 0.84150E 01, 0.76700E 01, 0.11310E 02,
      * 0.86760E 01, 0.78830E 01, 0.11846E 02, 0.89540E 01, 0.80630E 01,
      * 0.12293E 02, 0.92460E 01, 0.82120E 01, 0.12667E 02, 0.95470E 01,
      * 0.0, , 0.0, , 0.0, , -0.25556E-03, 0.54875E-02,
      * -0.16527E-03, 0.23493E-03, 0.11356E-01, 0.32042E-03, 0.14590E-02,
      * 0.11798E-01, 0.82102E-03, 0.16891E-02, 0.11629E-01, 0.12956E-02,
      * 0.21428E-02, 0.86783E-02, 0.20198E-02, 0.23782E-02, 0.69620E-02,
      * 0.25475E-02, 0.23619E-02, 0.57708E-02, 0.27283E-02, 0.19795E-02,
      * 0.48289E-02, 0.28715E-02, 0.16236E-02, 0.40369E-02, 0.29941E-02,
      * 0.13516E-02, 0.34077E-02, 0.30325E-02, 0.0, , 0.0, ,
      * 0.0, , 0.36619E-05, 0.25903E-05, 0.25014E-05, -0.12784E-05,
      * 0.34115E-05, 0.25451E-05, 0.13946E-03, 0.24256E-03, 0.16496E-03,
      * -0.37097E-05, -0.25071E-04, 0.15899E-05, 0.30618E-05, -0.64868E-05,
      * 0.28290E-05, 0.51733E-06, -0.37476E-05, 0.67945E-07, -0.31326E-05,
      * -0.29048E-05, 0.11945E-06, -0.18257E-05, -0.28476E-05, 0.22802E-06,
      * -0.12885E-05, -0.26141E-05, 0.92646E-07, -0.98218E-06, -0.25038E-05 /
0021 DATA x16/
      * -0.34925E-10, 0.0, , 0.0, , 0.0, , -0.80632E-08,
      * 0.17834E-06, -0.48627E-09, 0.51037E-07, -0.78710E-08, 0.34610E-10,
      * -0.27848E-04, -0.10383E-03, -0.13224E-04, 0.41190E-07, 0.68771E-07,
      * 0.13541E-07, -0.13900E-07, -0.13966E-07, -0.12714E-08, -0.39916E-08,
      * -0.14723E-07, 0.55730E-08, 0.81368E-08, -0.12029E-07, 0.39794E-08,
      * 0.30976E-09, -0.74182E-08, 0.25660E-08, -0.47721E-09, -0.35454E-08,
      * 0.66161E-09, -0.13392E-08, -0.27310E-08, 0.74990E-09, 0.0, ,
      * 0.0, , 0.0, /
0022 T=TX/1.8
0023 GO TO (10,20,30), KK
0024 1000 M=-1
0025 GO TO 50
0026 10 GO TO (11,11,12,11,11), K
0027 20 GO TO (13,13,12,13,13), K
0028 1003 M=-2
0029 GO TO 50
0030 30 GO TO (31,13,31,13,13), K
0031 31 M=-2
0032 GO TO 50
0033 11 IF ((T .LT. 100.) .OR. (T .GT. 600.)) GO TO 15
0034 T1= 100.
0035 T2= 110.0
0036 INC= 10
0037 IF (K .EQ. 4) GO TO 26
0038 NK= 52

```

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0039      GO TO 25
0040      12  IF ((T .LT. 298.15) .OR. (T .GT. 1500.)) GO TO 15
0041          T1= 298.15
0042          T2= 300.0
0043          INC= 100
0044          NK= 14
0045      GO TO 25
0046      13  IF ((T .LT. 100.) .OR. (T .GT. 1000.)) GO TO 15
0047          T1= 100.0
0048          T2= 200.0
0049          INC= 100
0050          NK= 11
0051      25  NK2= NK-2
0052          DO 28 II= 1,NK2
0053              T3= T2+INC
0054              IF (T3 .EQ. 300.) T3= 298.15
0055              IF ((T3 .EQ. 308.15) .OR. (T3 .EQ. 398.15)) T3= 300.
0056              IF ((T .GE. T1) .AND. (T .LT. T2)) GO TO 40
0057              T1= T2
0058              T2= T3
0059      28  CONTINUE
0060          II= NK-1
0061          GO TO 40
0062      26  NK= 51
0063          NK2= NK-2
0064          DO 27 II= 1,NK2
0065              T3= T2+INC
0066              IF ((T .GE. T1) .AND. (T .LT. T2)) GO TO 40
0067              T1= T2
0068              T2= T3
0069      27  CONTINUE
0070          II= NK-1
0071      40  GO TO (41,42,43), KK
0072      1001 H=-1
0073          GO TO 50
0074      41  TC= T-T1
0075          H= ((C1(K,II,4)*TC + C1(K,II,3))*TC + C1(K,II,2))*TC + C1(K,II,1)
0076          IF (K .EQ. 4) RETURN
0077          H= .18E04*H
0078          RETURN
0079      42  TC= T-T1
0080          H= ((C2(K,II,4)*TC + C2(K,II,3))*TC + C2(K,II,2))*TC + C2(K,II,1)
0081          RETURN
0082      43  TC= T-T1
0083          K= K-2
0084          IF (K .EQ. 0) K=1
0085          H= ((C3(K,II,4)*TC + C3(K,II,3))*TC + C3(K,II,2))*TC + C3(K,II,1)
0086          K= K-2
0087          IF (K .EQ. 3) K=2
0088          RETURN
0089      15  H= 0.0
0090      50  RETURN
0091      END

```


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0001      SUBROUTINE COEFF(COEF,ARRAY)
0002      DIMENSION ARRAY(72),MHA(72),M1(72),S1(72),CP1(72),MM1(72),
1          MM2(72),MM3(72),MHC(40)
0003      INTEGER CODE
0004      C      CHEMICAL * SENSIBLE ENTHALPHY FOR T > TI.
          DATA MM1/
19.2937814E+4 , 4.9679289 , 0.0 , 0.0 , , H
21.0650436E+5 , 4.9819292 , 0.0 , 0.0 , , O
31.7243891E+4 , 6.5117725 , 2.4740577E-4 , 0.0 , , OH
43.7810593E+4 , 7.7703187 , 1.3914575E-4 , 0.0 , , NO
5-4.9950257E+4 , 7.4991057 , 1.6384251E-4 , 0.0 , , CO
64.3795667E+2 , 6.2305090 , 2.7323736E-4 , 0.0 , , H2
7-270.5134204 , 6.8101302 , 2.8505033E-4 , 0.0 , , N2
8 -630.6330969 , 7.3851082 , 2.5992293E-4 , 0.0 , , O2
9-.0615 , 4.9682152 , 0.0 , 0.0 , , AR
A-175045.8247470 , 13.506027 , 0.0 , 0.0 , , CO2
B-.0615 , 4.9682152 , 0.0 , 0.0 , , NE
C-102632.3476190 , 7.1088046 , 7.678847E-4 , 0.0 , , H2O
O-1304.1576077 , 7.6123722 , 1.3657170E-4 , 0.0 , , N2
E-1240.9978428 , 7.8839888 , 1.5887864E-4 , 0.0 , , O2
F -0.02187 , 4.9681271 , 0.0 , 0.0 , , AR
G-177175.4038470 , 14.294766 , 0.0 , 0.0 , , CO2
H -0.02187 , 4.9681271 , 0.0 , 0.0 , , NE
I-104643.9857996 , 8.5658373 , 5.0418784E-4 , 0.0 , / H2O
0005      C      ENTROPY FOR T > TI.
          DATA MM2/
1 26.367556 , 5.3779781E-03,-0.9431089E-06, 0.7157248E-10, H
2 37.535609 , 5.4203862E-03,-0.9540069E-06, 0.7257386E-10, O
3 44.450387 , 5.2414646E-03,-0.4177444E-06, 0.0 , OH
4 48.070143 , 0.8479758E-02,-1.4094686E-06, 1.0545863E-10, NO
5 45.057500 , 0.8187987E-02,-1.3406214E-06, 0.951842E-10, CO
6 29.869398 , 0.7329605E-02,-1.2019850E-06, 0.9262449E-10, H2
7 57.275024 , -1.8300467E-02, 1.7559820E-05,-0.5815832E-08, N2
8 47.225630 , 0.7577402E-02,-0.8281940E-06, 0.0 , O2
9 36.446444 , 4.5571014E-03,-0.5119033E-06, 0.0 , AR
A 47.518398 , 1.1512786E-02,-1.2066643E-06, 0.0 , CO2
B 34.4116312 , 4.5570565E-03, -0.5118949E-06,0.0 , NE
C 43.261707 , 0.8244883E-02,-0.7782285E-06, 0.0 , H2O
D 46.856474 , 5.0506993E-03,-0.3700634E-06, 0.0 , N2
E 50.2049115 , 5.2780447E-03,-0.3852719E-06, 0.0 , O2
F 38.5124276 , 3.0262745E-03,-0.22832958E-6, 0.0 , AR
G 51.5035705 , 8.44472E-03 , -0.6170116E-06, 0.0 , CO2
H 34.8197332 , 4.5503522E-03,-0.6902733E-06, 0.0462520E-09, NE
I 45.6963147 , 0.6353274E-02,-0.115987E-06, 0.0 , / H2O
0006      C      SPECIFIC HEAT FOR T > TI.
          DATA MM3/
1 4.98615 , 0.0 , 0.0 , 0.0 , , H
2 5.0648570 , -4.9817011E-5, 0.7122534E-08, 0.0 , , O
3 6.1708494 , 0.6040710E-3, 0.4777281E-07,-1.4488393E-11, , OH
4 5.909456 , 1.9245802E-3, -0.4560416E-06, 0.3921985E-10, , NO
5 5.5732319 , 2.0076651E-3, -0.4552845E-06, 0.3777076E-10, , CO
6 9.6700579 , -4.3676505E-3, 2.526454E-06,-0.5547857E-09, , H2
7 5.7766562 , 1.5061552E-3, -2.0759936E-07, 0.0 , , N2
8 5.607584 , 2.7614501E-3, -0.8888113E-06, 1.0954859E-10, , O2
9 4.96815 , 0.0 , 0.0 , 0.0 , , AR
A 6.680396 , 0.5990060E-2, -1.7096379E-06, 0.1809910E-09, , CO2

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      B 4.96815      . 0.0      . 0.0      . 0.0      . NE
      C 7.1564387    . 0.9855705E-3, 0.4640690E-06, -1.0002320E-10, . H2O
      D 6.5727317    . 0.9099083E-3, -0.9596494E-07, . 0.0      . N2
      E 7.6813079    . 4.4281245E-4, -1.8738208E-08, . 0.0      . O2
      F 4.96815      . 0.0      . 0.0      . 0.0      . AR
      G 10.8521173   . 1.6107530E-3, -1.7125528E-07, . 0.0      . CO2
      H 4.96815      . 0.0      . 0.0      . 0.0      . NE
      I 5.9764766    . 2.5861179E-3, -2.3692669E-07, . 0.0      . H2O
C   SENSIBLE ENTHALPY COEFFICIENTS FOR T, LE. T1,900R-1800R,
C   1800R-2700R, 2700R-4000R.
0007 DATA M1/
      *272.57472     . 6.2849888     . 4.2460662E-4     . 0.0      . N2
      *49.9253121    . 6.7005911     . 4.6097941E-4     . 0.0      . O2
      * 0.19368      . 4.9682152     . 0.0      . 0.0      . AR
      *-291.6316413, 6.5377190, 28.320187E-4, . -0.3858033E-6, . CO2
      * 0.19368      . 4.9682152     . 0.0      . 0.0      . NE
      *356.6510897, 6.913576, 8.1349063E-4, . 0.0      . H2O
      *-220.5134204, 6.8101302, 2.8505033E-4, . 0.0      . N2
      *-630.6330969, 7.3851082, 2.5992293E-4, . 0.0      . O2
      *-0.0615       . 4.9681418     . 0.0      . 0.0      . AR
      *-3294.0760689, 11.07844, 5.4166925E-4, . 0.0      . CO2
      *-0.0615       . 4.9681418     . 0.0      . 0.0      . NE
      *152.8596437, 7.1089372, 7.6785528E-4, . 0.0      . H2O
      *-1304.1576077, 7.6123722, 1.3657170E-4, . 0.0      . N2
      *-1240.9978428, 7.8839888, 1.5887864E-4, . 0.0      . O2
      *-0.02187      . 4.9681271     . 0.0      . 0.0      . AR
      *-5537.3281389, 12.747913, 2.3106225E-4, . 0.0      . CO2
      *-0.02187      . 4.9681271     . 0.0      . 0.0      . NE
      *-1858.4935816, 8.5657282, 5.0420885E-4, . 0.0      . H2O
C   ENTROPY COEFFICIENTS FOR T, LE. T1,900R-1800R, 1800R-2700R,
C   2700R-4000R REVISED FQ.
0008 DATA S1/
      * 39.251394    . 0.0155587     . -0.5615997E-05, . 0.933764E-09, . N2
      * 42.269726    . 1.5770590E-02, -0.5390427E-05, . 0.8573795E-09, . O2
      *31.5883510     . 1.2918283E-02, -5.3921089E-06, . 0.9663917E-09, . AR
      * 41.78458      . 2.0871316E-02, -0.6347125E-05, . 0.9526361E-09, . CO2
      * 29.5537807    . 1.2917042E-02, -5.3907410E-06, . 0.9659557E-09, . NE
      * 37.437166     . 1.8092773E-02, -0.6382909E-05, . 1.0748317E-09, . H2O
      * 57.275024     . -1.8300467E-02, 1.7559820E-05, . -0.5815832E-09, . N2
      * 47.225630     . 0.7577402E-02, -0.828194E-06, . 0.0      . O2
      *36.4464480     . 4.5571014E-03, -0.5119033E-06, . 0.0      . AR
      * 47.518398     . 1.1512786E-02, -1.2066643E-06, . 0.0      . CO2
      *34.4116312     . 4.5570565E-03, -0.5118949E-06, . 0.0      . NE
      * 43.261707     . 0.8244883E-02, -0.7782285E-06, . 0.0      . H2O
      * 46.8564740     . 5.0506993E-03, -0.3700634E-06, . 0.0      . N2
      * 50.2049115     . 5.2780447E-03, -0.3852719E-06, . 0.0      . O2
      *38.5124276     . 3.0262745E-03, -0.22832958E-06, . 0.0      . AR
      * 51.5035705     . 8.44472E-03, -0.6170116E-06, . 0.0      . CO2
      *34.8197332     . 4.5503522E-03, -0.6902733E-06, . 0.0462520E-09, . NE
      * 45.6963147     . 0.6353274E-02, -0.4115987E-06, . 0.0      . H2O
C   SPECIFIC HEAT COEFFICIENTS FOR T, LE. T1,900R-1800R,
C   1800R-2700R, 2700R-4000R REV.
0009 DATA CP1/
      * 7.23667810   . -1.3015396E-03, 1.5759008E-06, -0.3746857E-09, . N2
      * 5.7846285     . 2.2415270E-03, -0.4580023E-06, . 0.0      . O2
      * 4.96815       . 0.0      . 0.0      . 0.0      . AR

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      • 5.3131429 • 0.8363827E-02,-0.3088999E-05, 0.4493104E-09 • C02
      • 4.96815 • 0.0 • 0.0 • 0.0 • NE
      • 7.5482768 • 4.2815697E-04, 0.7157717E-06, -1.3495489E-10 • M20
      • 5.7766562 • 1.5061552E-03,-2.0759936E-07, 0.0 • M2
      • 5.60758400 • 2.7614501E-03,-0.8888113E-06, 1.0954859E-10 • D2
      • 4.96815 • 0.0 • 0.0 • 0.0 • AR
      • 6.6803960 • 0.5990060E-02,-1.7096379E-06, 0.1809910E-09 • C02
      • 4.96815 • 0.0 • 0.0 • 0.0 • NE
      • 7.1564387 • 0.9855705E-03, 0.464069E-06,-1.0002320E-10 • M20
      • 6.5727317 • 0.9099083E-03,-0.9596494E-07, 0.0 • M2
      • 7.6813079 • 4.4281245E-04,-1.8738208E-08, 0.0 • D2
      • 4.96815 • 0.0 • 0.0 • 0.0 • AR
      • 10.8521173 • 1.6107530E-03,-1.7125528E-07, 0.0 • C02
      • 4.96815 • 0.0 • 0.0 • 0.0 • NE
      • 5.9764766 • 2.5861179E-03,-2.3692669E-07, 0.0 • M20
0010 C G1885 FREE ENERGY.
      DATA HMC/
      1 5.3150524E+04,-15.6253583 •-0.9767035E-03, 0.5610564E-07 • M
      2 6.0670223E+04,-21.8518477 •-0.9782325E-03, 0.5614114E-07 • O
      3 1.0843812E+04,-24.8213338 •-1.4149044E-03, 0.7304718E-07 • OM
      4 2.2896290E+04,-28.1298227 •-1.5979361E-03,0.8680263E-07 • NO
      5-2.5226419E+04,-26.3634922 •-1.5649177E-03, 0.8457005E-07 • CO
      6 1.4415362E+03,-17.8997838 •-1.3549595E-03, 0.6781319E-07 • M2
      7 1.2087000E+03,-25.6082461 •-1.5325905E-03, 0.8179650E-07 • M2
      8 1.2814893E+03,-27.3792772 •-1.6271943E-03, 0.8783605E-07 • D2
      9-9.2608408E+04,-27.9578811 •-2.5501816E-03, 1.3506145E-07 • C02
      A-5.6574736E+04,-25.0072600 •-1.8841889E-03, 0.8839907E-07/ • M20
0011 UD 1 1=1.72
0012 1 ARRAY(1) = 0.0
0013 GO TO(10,20,30,40,50,60,80,90).CODE
0014 10 DO 11 1=1.40
0015 11 ARRAY(1) = HMC(1)
0016 RETURN
0017 20 DO 21 1=1.72
0018 21 ARRAY(1) = HM1(1)
0019 RETURN
0020 30 DO 31 1=1.72
0021 31 ARRAY(1) = HM2(1)
0022 RETURN
0023 40 DO 41 1=1.72
0024 41 ARRAY(1) = HM3(1)
0025 RETURN
0026 50 DO 51 1=1.72
0027 51 ARRAY(1) = HMA(1)
0028 RETURN
0029 60 DO 61 1=1.72
0030 61 ARRAY(1) = M1(1)
0031 RETURN
0032 80 DO 81 1=1.72
0033 81 ARRAY(1) = S1(1)
0034 RETURN
0035 90 DO 91 1=1.72
0036 91 ARRAY(1) = CP1(1)
0037 RETURN
0038 END

```

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CCC

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```

0001      FUNCTION CCC(M,N,T)
          C      TEMPERATURE T IS IN DEGREES R
          C      N2 -1,10,15, 02-2,20,25, AR-3,30,35, CO2-4,40,45, NE-5,50,55
0002      GO TO(100,200,300),M
0003      100 GO TO(1,2,3,4,5),N
          C      3ND VIRIAL COEFFICIENT(C)- AEDC- TR-71-39.
0004      1 CCC = (3.5528210 -4.7253632E-02 *T)/(1.0 -4.7446815E-03 *T)
0005      GO TO 1000
0006      2 CCC = (-4.2345758E+01)/(1.0 -0.9728086E-02 *T)
0007      GO TO 1000
0008      3 CCC = (((-1.0787834E-07 *T) + 2.4336141E-04) * T -
          1      0.19016416) * T + 59.879538
0009      GO TO 1000
0010      4 CCC = 115.17385 -0.1338398 * T + 0.3190838E-4 * T * T
0011      GO TO 1000
0012      5 CCC = 0.0
0013      GO TO 1000
0014      200 GO TO(10,20,30,40,50),N
          C      T(OC/OT)
0015      10 CCC = (-30.396628E-03 *T)/(((22.5120025E-06 *T)-9.4893630E-03)
          1 * T + 1.0)
0016      GO TO 1000
0017      20 CCC = (4.1194317E-03 *T)/(1.0 - 0.9728086E-02 *T)
0018      GO TO 1000
0019      30 CCC = (((-3.2363502E-07 * T) + 4.8672282E-04) * T
          1      -0.19016416) * T)
0020      GO TO 1000
0021      40 CCC = 0.1338398 * T + 0.6381676E-4 * T * T
0022      GO TO 1000
0023      50 CCC = 0.0
0024      GO TO 1000
0025      300 GO TO(15,25,35,45,55),N
          C      T**(D**C/OT**)
0026      15 CCC = -28.8444637E-05 * T * T + 136.8577931E-08 * T **3/
          1(1.0-9.4893630E-3 * T + 22.5120025E-6 * T *T) ** 2
0027      GO TO 1000
0028      25 CCC = (-4.0074185E-05 * T * T) / (1.0 -0.9728086E-02 *T)
0029      GO TO 1000
0030      35 CCC = 4.8672282E-04 *T *T -6.4727004E-07 *T *T *T
0031      GO TO 1000
0032      45 CCC = 0.6381676E-4 * T * T
0033      GO TO 1000
0034      55 CCC = 0.0
0035      1000 CCC = CCC * 100.0
0036      RETURN
0037      END

```

FORTRAN IV G LEVEL 21

SONV

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```

0001      SUBROUTINE SONV(WTM,F,T,CP,G,A)
          C      TEMPERATURE T MUST BE IN DEGREES R
          C      SUBROUTINE TO CALCULATE SONIC VELOCITY
0002      IF(F.EQ.0)WTM=28.9646
0003      G = CP/(CP-(1.987165/WTM))
0004      X = 32.16 * 1.987165 * 1054.3502645/ 1.3558179
0005      A = (ABS((G*X*T)/WTM))**0.5
0006      RETURN
0007      ENO

```

FORTRAN IV G LEVEL 21

888

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```

0001      FUNCTION 888(M,N,T)
          C      TEMPERATURE T IS IN DEGREES R
          C      M2 -1,10,15, 02-2,20,25, AR-3,30,35, CO2-4,40,45, NE-5,50,55
0002      GO TO(100,200,300),M
0003      100 GO TO(1,2,3,4,5),N
          C      2ND VIRIAL COEFFICIENT(B) - AE0C - TR-71-39.
0004      1 888 = (((-0.3534783E-03 * T) - 0.6636132) * T + 5.1364637E+02)
          1 / (((-0.9296798E-05) * T - 1.7158299E-02) * T + 1.0)
0005      GO TO 1000
0006      2 888 = (((-1.5050447E-04 * T) - 4.7667818E-01) * T + 4.2857084E+02)
          1 / (((-0.5095962E-05 * T) - 1.4123010E-02) * T + 1.0)
0007      GO TO 1000
0008      3 888 = ((((-1.4860291E-08 * T) + 0.4772262E+03) * T -
          1 0.8705351) * T + 3.8904656E+02) / (((1.4973286E-10 *
          2 T) + 1.1790085E-05) * T - 1.4845725E-02) * T + 1.0)
0009      GO TO 1000
0010      4 888 = (((0.7026469E-04 * T) - 5.0336843E-01) * T + 5.3152906E+02)
          1 / (((-2.2018674E-08 * T) - 0.6113584E-02) * T + 1.0)
0011      GO TO 1000
0012      5 888 = (59.425695 - 0.2714498 * T) / (1.0 - 1.6463468E-02 * T)
0013      GO TO 1000
0014      200 GO TO(10,20,30,40,50),N
          C      T(08/DT)
0015      10 888 = (-3.4560792E+02) / (((-0.29627746E-05 * T) - 1.1286423E-02)
          1 * T + 1.0)
          GO TO 1000
0016      20 888 = (-3.1691728E+02) / (((0.4514126E-09 * T) - 0.3228332E-05)
          1 * T - 0.9521198E-02) * T + 1.0)
          GO TO 1000
0017      30 888 = (-2.7524532E+02 + 4.4273617E-02 * T) / (1.0 -
          1 0.9485511E-02 * T)
          GO TO 1000
0018      40 888 = (((((18.9162693E-12 * T) - 7.8788948E-09) * T
          1 - 0.9807759E-03) * T + 5.3458176) * T) / ((((-7.1340504E-08
          2 * T) - 1.104452E-02) * T + 1.0) ** 2)
          GO TO 1000
0019      50 888 = (-6.1992870E+01 + 1.8886040E-02 * T) / (1.0 - 1.7014989E-02 * T)
          GO TO 1000
0020      300 GO TO(15,25,35,45,55),N
          C      T**(D**8/DT**8)
0021      15 888 = (6.7503388E+02) / (((1.3834608E-09 * T) - 0.4815325E-05)
          1 * T - 0.8951382E-02) * T + 1.0)
          GO TO 1000
0022      25 888 = (((((0.3089713E-09 * T) - 0.7888087E-05) * T + 1.0935667E-02)
          1 * T - 4.9627303) * T - 3.3796998 * 01) / (((0.9466770E-10
          2 * T) - 0.2105136E-06) * T + 1.2893683E-04) * T
          3 - 1.9686162E-02) * T + 1.0)
          GO TO 1000
0023      35 888 = (3.9858659E+02 - 3.4251675E-02 * T) / (1.0 + 0.6811836E-02 * T)
          GO TO 1000
0024      45 888 = (((((-50.1159356E-16 * T) - 47.4547667E-13) * T
          1 - 1.4462917E-07) * T - 125.9326564E-05) * T
          2 + 11.8074171 * T * T) / ((((-7.13405040E-08 * T)
          3 - 1.104452E-02) * T + 1.0) ** 4)
          GO TO 1000
0025      55 888 = (1.5852079E+02 - 3.1378493E-02 * T) / (1.0 - 1.8918656E-02 * T)
0026      1000 RETURN
          ENH
0027
0028
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0030
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NOMENCLATURE

A^*	(See Eq. (19))
$a-l$	Coefficients for equations
B^*	(See Eq. (20))
B	Second virial coefficient, cm^3/mole
C	Third virial coefficient, cm^6/mole
C_p	Specific heat at constant pressure, $\text{Btu}/\text{lbm-mole-}^\circ\text{R}$
c_p	Specific heat at constant pressure, $\text{Btu}/\text{lbm-}^\circ\text{R}$
f	Fuel-to-air ratio, $\text{lbm}_{\text{fuel}}/\text{lbm}_{\text{air}}$
H	Enthalpy, $\text{Btu}/\text{lbm-mole}$
h	Enthalpy, Btu/lbm
MW	Molecular weight, $\text{lbm}/\text{lbm-mole}$
m	Fuel, hydrogen-to-carbon weight ratio, $\text{lbm}_H/\text{lbm}_C$
n	Mole fraction, moles/mole
P	Pressure, psia
R	Gas constant
S	Entropy, $\text{Btu}/\text{lbm-mole}^\circ\text{R}$
s	Entropy, $\text{Btu}/\text{lbm}^\circ\text{R}$
T	Temperature, $^\circ\text{R}$
V	Specific volume, cm^3
XM	Number of hydrogen atoms in a mole of hydrogen fuel
XN	Number of carbon atoms in a mole of hydrocarbon fuel
η	Efficiency

SUBSCRIPTS

a	Pressure in atmospheres
B	Base temperature
eq	Equilibrium

I	Value where the effects of chemical dissociation are first considered
i	Constituent
j, k, m, n	Property coefficients
p	Pressure
T	Temperature, °R
u	Universal